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**SIMPLIFIED METHOD FOR SOLVING PROBLEMS
INVOLVING CHEMICALLY REACTING
ONE-DIMENSIONAL FLOW**

I. T. Osgerby

ARO, Inc.

March 1969

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ARNOLD ENGINEERING DEVELOPMENT CENTER
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FOREWORD

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This technical report has been reviewed and is approved.

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ABSTRACT

A simplified technique for solving "stiff" differential equations common to chemically reacting quasi-one-dimensional inviscid non-equilibrium flow analyses is presented. The method is basically that used by Degroat and Abbett with the generalization made to allow for a prescribed area distribution rather than the constant pressure (and hence constant velocity) process assumed by them. In addition, the equations are written for hydrogen/air combustion rather than methane/air. The advantage of the technique is that the chemical kinetic calculations can be solved quickly without loss of accuracy, and thus can be relegated to the status of a subroutine in complicated fluid-dynamic problems.

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NOMENCLATURE

A	Area, cm^2
$A_i, B_i, C_i,$ D_i, E_i	Coefficients in specific enthalpy equations
$a_{i,k}, c_i$	Coefficients in linearized species equations
b, c	Constants in an integration step
b_j	Backward reaction rate for the jth reaction, $\text{cm}^3/\text{mole sec}$ or $\text{cm}^6/\text{mole}^2\text{sec}$
C_p	Specific heat, $\text{cal}/\text{gm } ^\circ\text{K}$
f_j	Forward reaction rate for the jth reaction, $\text{cm}^3/\text{mole sec}$ or $\text{cm}^6/\text{mole}^2\text{sec}$
H	Static enthalpy of the mixture, cal/gm
H_0	Total enthalpy of the mixture, cal/gm
h_i	Specific enthalpy of ith species, cal/gm
M_i	Molecular weight of the ith species, gm/mole
\dot{m}	Mass flow rate, gm/sec
N	Total number of reactions
n_A	Number of rapidly varying species
n_T	Total number of species
p	Pressure, atm
R	Universal gas constant, $\text{cm}^3 \text{ atm}/\text{mole } ^\circ\text{K}$

$R_{kj}, R^{\circ}_{kj},$ R_{ij}	Coefficients in linearized species equations
S_{ij}	Coefficients in linearized species equations
T	Temperature, °K
u	Velocity, cm/sec
x	Distance along duct, cm
Y	Sum of species concentrations $\left(Y = \sum_{i=1}^n y_i \right)$, moles/cm ³
y_i	Concentration of ith species, moles/cm ³
\dot{y}_i	Rate of change of the concentration of the ith species, moles/cm ³ sec
\dot{y}_{ij}	Rate of change of the concentration of the ith species in the jth reaction, moles/cm ³ sec
α_i	Mass fraction of the ith species, gm/gm
β	Coefficient in area equation
γ_i	Concentration of ith species, moles/gm
δ	Coefficient in species equation, 1/cm
ν	Stoichiometric coefficient
ρ	Density, gm/cm ³
ψ	Coefficient in linearized species equations

SUBSCRIPT

c	Computed value of variable at the end of an integration interval
-----	--

SUPERSCRIPT

$^{\circ}$	Value of variable at the beginning of an integration interval
$-$	Variable divided by 1000

SECTION I INTRODUCTION

Analysis of gaseous flow fields in which the gas is not in chemical equilibrium consists of point by point evaluation of the gas composition and fluid-dynamic variables. Formal analysis involves the integration of a set of coupled, first-order, ordinary, nonlinear, stiff, differential equations. Numerical solution of these equations often eludes the computer when sought by classical means and at best requires considerable computation time. The primary reason equations of this class (stiff) present such difficulties is that an exceedingly small integration step-size is sometimes required, making classical integration techniques impractical even on the most sophisticated computing machines. Various works have been published on this subject (Refs. 1 through 7). The method of solution described in this report represents a combination of some of the improvements made in several of the above references, notably Refs. 5 and 6. In this method the stiffness and non-linearity are removed entirely by using approximation techniques. Large integration stepsizes become possible with this method, particularly for near-equilibrium flows.

SECTION II BASIC EQUATIONS

Let y_i be the concentration of species i (moles/cm³) and M_i be its molecular weight. Then

$$y_i = \rho \frac{\alpha_i}{M_i} \quad (1)$$

where α_i is the mass fraction of species i and ρ is the mixture density.

At any instant of time, the rate of change of the concentration of species i in reaction j is given by the general formula:

$$\dot{y}_{ij} = f_j \prod y_k^{\nu_k'} - b_j \prod y_k^{\nu_k''} \quad (2)$$

where ν_k' and ν_k'' are either zeros or integers, and the factors f_j and b_j are forward and backward reaction rate coefficients for the j th reaction, and are functions of temperature only. The total rate of change of the concentration of species i caused by all the chemical reactions is given by the following species continuity equation:

$$\dot{y}_i = \sum_{j=1}^N \dot{y}_{ij} = F_i(T, y_1, y_2, \dots, y_{N_T}) \quad (3)$$

Suppose that in an integration step, the variation of T is negligible, then an analytical solution to Eqs. (3) can be obtained:

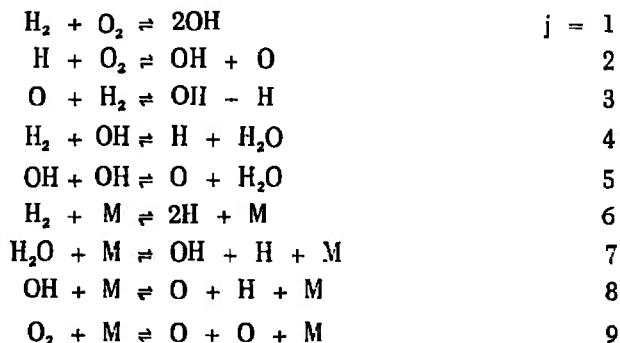
$$y_i = y_i(t) \quad (4)$$

However, Eqs. (3) are nonlinear and thus it is not possible to integrate them directly. Now, if Eqs. (3) are linearized by dropping higher order terms which may be assumed to be negligibly small in an integration step, then an exact analytical solution can be obtained over an integration interval. This has been done (Ref. 5) and with certain other modifications (described in detail later) the concentration can be obtained as a function of distance (x) also: $y_i = y_i(x)$.

Since the solution is obtained in closed form over an integration interval, no stability problems arise. The advantage of this technique stems from the fact that the integration interval stepsize in the linearized system can be several orders of magnitude greater than in the original system. In the next sections, a specific example is examined in detail.

SECTION III COMBUSTION OF HYDROGEN IN AIR

Let air be represented by a mixture of nitrogen and oxygen. The nitrogen is considered inert and the oxygen can dissociate or react with hydrogen. Six species are considered in the chain reaction combustion model: H , O , H_2O , OH , O_2 , and H_2 , which are numbered one through six. The inert nitrogen is numbered seven for summation purposes in computing the third body M for third-order reactions. The reactions considered representative for combustion of hydrogen in air at high temperatures are (Ref. 5):



Equations (2) are:

$$\begin{aligned}
 \dot{y}_{41} &= 2f_1 y_5 y_6 \\
 \dot{y}_{22} &= f_2 y_1 y_5 - b_2 y_2 y_4 \\
 \dot{y}_{13} &= f_3 y_2 y_6 - b_3 y_1 y_4 \\
 \dot{y}_{14} &= f_4 y_4 y_6 - b_4 y_1 y_3 \\
 \dot{y}_{25} &= f_5 y_4^2 - b_5 y_2 y_3 \\
 \dot{y}_{16} &= 2f_6 y_6 Y - 2b_6 y_1^2 Y \\
 \dot{y}_{17} &= f_7 y_3 Y - b_7 y_1 y_4 Y \\
 \dot{y}_{18} &= f_8 y_4 Y - b_8 y_1 y_2 Y \\
 \dot{y}_{29} &= 2f_9 y_5 Y - 2b_9 y_2^2 Y
 \end{aligned} \tag{5}$$

$$\begin{array}{ccccccc}
 i = & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
 & H & O & H_2O & OH & O_2 & H_2 & N_2
 \end{array}$$

where

$$Y = \sum_{i=1}^7 y_i \tag{6}$$

The f_j and b_j are given in Appendix II.

Equations (3) are obtained from the following:

$$\begin{array}{lll}
 \dot{y}_{11} = 0 & \dot{y}_{21} = 0 & \dot{y}_{31} = 0 \\
 \dot{y}_{12} = -\dot{y}_{22} & \dot{y}_{22} = \dot{y}_{22} & \dot{y}_{32} = 0 \\
 \dot{y}_{13} = \dot{y}_{13} & \dot{y}_{23} = -\dot{y}_{13} & \dot{y}_{33} = 0 \\
 \dot{y}_{14} = \dot{y}_{14} & \dot{y}_{24} = 0 & \dot{y}_{34} = \dot{y}_{14} \\
 \dot{y}_{15} = 0 & \dot{y}_{25} = \dot{y}_{25} & \dot{y}_{35} = \dot{y}_{25} \\
 \dot{y}_{16} = \dot{y}_{16} & \dot{y}_{26} = 0 & \dot{y}_{36} = 0 \\
 \dot{y}_{17} = \dot{y}_{17} & \dot{y}_{27} = 0 & \dot{y}_{37} = -\dot{y}_{17} \\
 \dot{y}_{18} = \dot{y}_{18} & \dot{y}_{28} = \dot{y}_{18} & \dot{y}_{38} = 0 \\
 \dot{y}_{19} = 0 & \dot{y}_{29} = \dot{y}_{29} & \dot{y}_{39} = 0 \\
 \dot{y}_{41} = \dot{y}_{41} & \dot{y}_{51} = -\dot{y}_{41}/2 & \dot{y}_{61} = -\dot{y}_{41}/2 \\
 \dot{y}_{42} = \dot{y}_{22} & \dot{y}_{52} = -\dot{y}_{22} & \dot{y}_{62} = 0 \\
 \dot{y}_{43} = \dot{y}_{13} & \dot{y}_{53} = 0 & \dot{y}_{63} = -\dot{y}_{13} \\
 \dot{y}_{44} = -\dot{y}_{14} & \dot{y}_{54} = 0 & \dot{y}_{64} = -\dot{y}_{14} \\
 \dot{y}_{45} = -2\dot{y}_{25} & \dot{y}_{55} = 0 & \dot{y}_{65} = 0 \\
 \dot{y}_{46} = 0 & \dot{y}_{56} = 0 & \dot{y}_{66} = -\dot{y}_{16}/2 \\
 \dot{y}_{47} = \dot{y}_{17} & \dot{y}_{57} = 0 & \dot{y}_{67} = 0 \\
 \dot{y}_{48} = -\dot{y}_{18} & \dot{y}_{58} = 0 & \dot{y}_{68} = 0 \\
 \dot{y}_{49} = 0 & \dot{y}_{59} = -\dot{y}_{29}/2 & \dot{y}_{69} = 0
 \end{array}$$

$$\dot{y}_i = \sum_{j=1}^9 \dot{y}_{ij} \quad i = 1,6 \quad (7)$$

The following two equations are obtained as linear combinations of Eqs. (7)

$$\begin{aligned} 2\dot{y}_6 + \dot{y}_1 + \dot{y}_4 + 2\dot{y}_5 &= 0 \\ 2\dot{y}_5 + \dot{y}_2 + \dot{y}_4 + \dot{y}_3 &= 0 \end{aligned} \quad (8)$$

These equations express the conservation of the number of atoms of hydrogen and oxygen.

The following additional equations must be added to make the problem determined.

3.1 CONSERVATION OF SPECIES

$$\rho u \frac{d\alpha_i}{dx} = M_i \dot{y}_i \quad (9)$$

where d/dx means substantial derivative and u is the flow velocity.

3.2 GLOBAL CONTINUITY

$$\rho u A = \dot{m} = \text{constant} \quad (10)$$

where A is the flow area and \dot{m} is the mass flow rate.

3.3 MOMENTUM EQUATION

$$\frac{dp}{dx} + \rho u \frac{du}{dx} = 0 \quad (11)$$

where p is the static pressure.

3.4 ENERGY EQUATION

$$H_o = h + \frac{u^2}{2} = \text{constant} \quad (12)$$

where H is the static enthalpy of the gas mixture and includes sensible and chemical energies, H_0 is the total enthalpy.

$$H = \sum_{i=1}^7 a_i h_i \quad (13)$$

where h_i is the sensible enthalpy of species i . These partial enthalpies are defined through partition functions of the species which are functions of temperature. For practical purposes, piecewise parabolic fits can be obtained by curve fitting data such as are tabulated in Ref. 8 thus:

$$h_i = A_i + B_i T + C_i (T - T_{0i})^2 \quad (14)$$

where A_i , B_i , and C_i are polynomial coefficients and T_{0i} is a reference temperature. Details are given in Appendix III.

3.5 STATE EQUATION

$$p = RT \sum_{i=1}^7 y_i \quad (15)$$

where R is the universal gas constant.

SECTION IV LINEARIZED EQUATIONS FOR THE CONCENTRATIONS

The mass fractions (α_i) can be eliminated by means of Eq. (1).

Let

$$y_i = \frac{\alpha_i}{M_i} \quad (16)$$

$$\therefore y_i = \rho \gamma_i \quad (17)$$

From Eq. (9)

$$\frac{dy_i}{dx} = \frac{1}{\rho u} \dot{y}_i \quad (18)$$

From Eq. (10)

$$\frac{dy_i}{dx} = \left(\frac{\dot{m}}{A}\right)^{-1} \dot{y}_i \quad (19)$$

In every computational step, the following simplifying assumptions are made:

1. The reaction rate coefficients f_j and b_j are constant throughout a step.

2. The logarithm of the density is a linear function of distance throughout a step. Consequently, a parameter

$$\delta = \frac{1}{\rho} \frac{d\rho}{dx} \quad (20)$$

constant throughout a step, can be introduced. Hence if ρ^0 is the initial value of the density in a step and ρ_c is the final value, the ratio $\psi = \rho_c/\rho^0$ is given by

$$\psi = \rho_c/\rho^0 \approx 1 + \delta \Delta x \quad (21)$$

3. The sum of the concentrations Y is also constant throughout a step.

Now Eqs. (5) and (7) can be used to eliminate the terms \dot{y}_i in Eqs. (19). The result is a system of ordinary differential equations in the concentrations which can be solved if the area (A) is given as a function of x . An attempt can be made to solve these equations in closed form throughout a step.

First, Eqs. (8) can be used to eliminate two of the concentrations. The slowly varying concentrations O_2 and H_2 are chosen. Differentiating Eq. (1) yields

$$\frac{dy_i}{dx} = \frac{a_i}{M_i} \frac{d\rho}{dx} + \frac{\rho}{M_i} \frac{da_i}{dx} \quad (22)$$

and using Eq. (9)

$$\frac{dy_i}{dx} = \frac{1}{\rho} \frac{d\rho}{dx} y_i + \frac{1}{u} \dot{y}_i \quad (23)$$

$$= \frac{1}{u} \dot{y}_i + \delta y_i \quad (24)$$

Thus using Eqs. (8) and (24) one can obtain

$$y_5 = - \frac{y_2 + y_3 + y_4}{2} + \psi \left\{ y_5^0 + \frac{y_2^0 + y_3^0 + y_4^0}{2} \right\}$$

$$y_6 = - \frac{y_1 + y_4}{2} - y_3 + \psi \left\{ y_6^0 + y_3^0 + \frac{y_1^0 + y_4^0}{2} \right\} \quad (25)$$

where $()^0$ means initial value at the beginning of the step.

$$\text{Let } b = \psi \left\{ y_5^0 + \frac{y_2^0 + y_3^0 + y_4^0}{2} \right\}$$

$$\text{and } c = \psi \left\{ y_6^0 + y_3^0 + \frac{y_1^0 + y_4^0}{2} \right\} \quad (26)$$

Equations (25) and (26) can be restated:

$$\begin{aligned} \dot{y}_3 &= b - \frac{y_2 + y_3 + y_4}{2} \\ \dot{y}_6 &= c - \frac{y_1 + y_4}{2} - y_3 \end{aligned} \quad (27)$$

At this stage, the expressions (Eqs. (27)) for y_5 and y_6 can be substituted into Eqs. (5) and the results used in the first four rows of Eqs. (7). Therefore, \dot{y}_1 , \dot{y}_2 , \dot{y}_3 , and \dot{y}_4 , now depend only on the variables y_1 , y_2 , y_3 , y_4 , and δ and contain a number of constant coefficients defined by the values of T and of each concentration at the beginning of an integration step. If Eqs. (19) are used with $i = 1, 4$; $\delta = \frac{1}{\rho} \frac{d\rho}{dx}$, the y_i described previously and a known area distribution, a system of four ordinary differential equations in the four unknowns y_1 , y_2 , y_3 , and y_4 is obtained with x as the independent variable. These equations have the general form

$$\frac{dy_i}{dx} = F_i(y_k, \delta, A) \quad i, k = 1, 4 \quad (28)$$

where the $F_i(y_k, \delta, A)$ are linear combinations of constant terms, first-order terms, and second-order terms in y_k . The value of δ to be used, described later, does not complicate the system since it is assumed constant throughout a step.

A system such as Eqs. (28) cannot be solved in closed form, but can be easily reduced to a linear system by writing

$$y_i y_k = - y_i^0 y_k^0 + y_i^0 y_k + y_k^0 y_i \quad (29)$$

After substitution of all the terms $y_i y_k$ with Eq. (29), the system of Eqs. (28) is approximated by the linear system

$$\frac{dy_i}{dx} = \left(\frac{\dot{m}}{A} \right)^{-1} \left[\sum_{k=1}^4 a_{i,k} y_k + c_i \right] \quad i = 1, 4 \quad (30)$$

Appendix IV gives the expressions for the constant coefficients $a_{i,k}$ and c_i .

Several methods may be used to solve Eqs. (30).

4.1 METHOD OF MORRETTI (REF. 5)

In this analysis of hydrogen/air combustion the velocity was not a variable and hence Eq. (24) is solved instead of Eq. (30):

$$\frac{dy_i}{dt} = \dot{y}_i + \delta y_i \quad i = 1, 4 \quad (31)$$

A solution to this set of equations is

$$y_i = \sum_{k=1}^4 \lambda_{i,k} e^{r_k \Delta t} \quad (32)$$

where the eigenvalues r_k are the roots of the characteristic equation

$$a_{i,k} - r_k \delta_{i,k} = 0 \quad (33)$$

the $\lambda_{i,k}$ are the corresponding eigen functions and $\delta_{i,k}$ is Kronecker's delta. In general, the roots r_k may be complex which increases the difficulty of obtaining the exact solution to the point where it renders that method impractical when more than four species are considered.

4.2 METHOD OF DEGROAT AND ABBETT (REF.6)

Again a constant velocity system was considered though the species considered corresponded to combustion of methane. An approximate solution to Eq. (31) is assumed

$$y_i = \sum_{q=0}^2 d_{iq} t^q \quad (34)$$

This solution is substituted into both sides of Eq. (31) and a residue is defined as follows:

$$\begin{aligned} R_i(t) &= \frac{dy_i}{dt} - \dot{y}_i - \delta y_i \\ &= \sum_{q=1}^2 q d_{iq} t^{q-1} - \sum_{q=0}^2 \sum_{k=1}^{n_A} a_{ik} d_{kq} t^q - c_i \end{aligned} \quad (35)$$

Requiring that

$$\int_0^{\frac{\Delta t}{2}} R_i(t) dt = \int_{\frac{\Delta t}{2}}^{\Delta t} R_i(t) dt = 0 \quad (36)$$

yields the two additional conditions required for the evaluation of the d_{iq} , d_{kq} for each equation

$$\sum_{q=1}^2 \left[d_{iq} t^q - \sum_{k=1}^{n_A} \frac{a_{ik} d_{kq} t^{q+1}}{q+1} \right]_0^{\frac{\Delta t}{2}} - \left[\sum_{k=1}^{n_A} a_{ik} d_{k0} t - c_{it} \right]_0^{\frac{\Delta t}{2}} = 0$$

$$\sum_{q=1}^2 \left[d_{iq} t^q - \sum_{k=1}^{n_A} \frac{a_{ik} d_{kq} t^{q+1}}{q+1} \right]_{\frac{\Delta t}{2}}^{\Delta t} - \left[\sum_{k=1}^{n_A} a_{ik} d_{k0} t - c_{it} \right]_{\frac{\Delta t}{2}}^{\Delta t} = 0 \quad (37)*$$

Simplifying,

$$\sum_{q=1}^2 \left[d_{iq} \left(\frac{\Delta t}{2} \right)^q - \sum_{k=1}^{n_A} \frac{a_{ik} d_{kq}}{q+1} \left(\frac{\Delta t}{2} \right)^{q+1} \right] - \sum_{k=1}^{n_A} a_{ik} d_{k0} \left(\frac{\Delta t}{2} \right) - b_i \frac{\Delta t}{2} = 0$$

$$\sum_{q=1}^2 \left[d_{iq} (\Delta t)^q \left(\frac{2^q - 1}{2^q} \right) - \sum_{k=1}^{n_A} \frac{a_{ik} d_{kq}}{q+1} (\Delta t)^{q+1} \left(\frac{2^{q+1} - 1}{2^{q+1}} \right) \right]$$

$$- \sum_{k=1}^{n_A} a_{ik} d_{k0} \left(\frac{\Delta t}{2} \right) - c_i \left(\frac{\Delta t}{2} \right) = 0 \quad (38)$$

where n_A is the number of rapidly varying species (see Eq. (25)).

There results a set of $2n_A$ linear algebraic equations for the $2n_A$ unknown terms. The algebraic equations are then solved by a maximum pivotal point matrix reduction method. The d_{iq} being known, an explicit solution is given for each species over the time interval considered.

4.3 EXTENSION OF METHODS 1 AND 2 TO VARIABLE VELOCITY SYSTEMS

A solution to Eq. (30) is assumed to be given by

$$y_i = \sum_{q=0}^2 d_{iq} x^q \quad (39)$$

Substitute into Eq. (30)

$$\frac{dy_i}{dx} = \left(\frac{\dot{m}}{A} \right)^{-1} \left[\sum_{q=0}^2 \sum_{k=1}^{n_A} a_{ik} d_{kq} x^q + c_i \right] \quad (40)$$

*The inner summation on $a_{ik} d_{kq}$ is written outside the brackets in Ref. 6 which, if taken literally, would lead to erroneous results.

Differentiating Eq. (17)

$$\begin{aligned}\frac{dy_i}{dx} &= \frac{1}{\rho} \left[\frac{dy_i}{dx} - \delta y_i \right] \\ &= \frac{1}{\rho^\circ e^{\delta x}} \left[\sum_{q=1}^2 q d_{iq} x^{q-1} - \delta \sum_{q=0}^2 d_{iq} x^q \right]\end{aligned}\quad (41)$$

A new residue is defined as

$$\begin{aligned}R_i(x) &= \frac{1}{\rho} \left[\frac{dy_i}{dx} - \delta y_i \right] - \frac{dy_i}{dx} \\ R_i(x) &= \frac{1}{\rho^\circ e^{\delta x}} \left[\sum_{q=1}^2 q d_{iq} x^{q-1} - \delta \sum_{q=0}^2 d_{iq} x^q \right] \\ &\quad - \left(\frac{\dot{m}}{A} \right)^{-1} \left[\sum_{q=0}^2 \sum_{k=1}^{n_A} a_{ik} d_{kq} x^q + c_i \right]\end{aligned}\quad (42)$$

If the area (A) is specified as a function of x in the interval, then integration of the residual can be carried out:

$$\begin{aligned}\int_0^{\frac{\Delta x}{2}} R_i(x) dx &= 0 \\ \int_{\frac{\Delta x}{2}}^{\Delta x} R_i(x) dx &= 0\end{aligned}\quad (43)$$

and again a set of $2 n_A$ linear algebraic equations is obtained which can be solved by standard matrix methods.

The unknown parameter δ is required to enable the unknown d_{iq} terms to be evaluated via Eqs. (43). There is no way in which δ can be calculated directly, hence an iterative solution is required. A simple test is used to verify whether the assumed value of δ is compatible with the changes in species concentration calculated from a solution to Eqs. (43). The temperature at the end of the integration interval can be obtained from two independent equations: (a) equation of state, and (b) energy equation.

- a. The pressure (p_c) at the end of an interval is obtained from a solution of the continuity and momentum equations

$$\frac{dp}{dx} = \frac{1}{\rho} \left(\frac{\dot{m}}{A} \right)^2 \left[\frac{1}{A} \frac{dA}{dx} + \frac{1}{\rho} \frac{d\rho}{dx} \right] \quad (44)$$

Since A is specified as a function of x in an interval Eq. (23) can be integrated after making the substitutions

$$\rho = \rho^o e^{\delta x} \text{ and } \frac{1}{\rho} \frac{d\rho}{dx} = \delta$$

From the equation of state

$$T_c = p_c \left\{ \frac{1}{R Y} \right\} \quad (45)$$

The value of p_c is obtained from integration of Eq. (44).

b. The enthalpy at the end of an interval is given by

$$\begin{aligned} H_c &= H_o - \frac{u_c^2}{2} \\ &= \sum_{i=1}^n \alpha_i h_i = \frac{1}{\rho} \sum_{i=1}^7 y_i M_i h_i \end{aligned} \quad (46)$$

From Eq. (14) $h_i = A_i + B_i T + C_i (T - T_{oi})^2$

From the continuity equation

$$\dot{m} = \rho u A \quad \therefore u_c = \frac{\dot{m}}{\rho_c A_c} \quad (47)$$

If the expressions for ρ and A as functions of x are inserted in Eq. (47) and the value of u_c substituted in Eq. (46) a quadratic expression in T is obtained:

$$A^* T_c^2 - 2B^* T_c + C^* = H_o - \frac{u_c^2}{2} \quad (48)$$

$$A^* T_c^2 - 2B^* T_c + C^* - \left\{ H_o - \frac{u_c^2}{2} \right\} = 0 \quad (49)$$

which can be solved for T_c . The terms A^* , B^* , and C^* are defined in Appendix III.

The values of T_c obtained in Eqs. (45) and (49) should agree. If they do not a new δ is assumed and the calculation for species composition and temperature is repeated. A Newton-Raphson iteration procedure for compatible values of δ and T has been found to be quite adequate and usually takes no more than three iterations to obtain a good solution.

Having solved for the new concentrations y_1 , y_2 , y_3 , and y_4 , we obtain the new values of y_5 and y_6 from Eqs. (27).

4.4 COMPUTATION OF DENSITY

Density is defined by

$$\rho = \sum_{i=1}^{n_T} y_i M_i \quad (50)$$

Now the mass fraction of the inert species ($N_2 = \alpha_7$) does not change; therefore,

$$\rho_c = \left\{ \frac{1}{1 - \alpha_7} \right\} \sum_{i=1}^6 y_i M_i \quad (51)$$

4.5 COMPUTATION OF VELOCITY

A new velocity is obtained from the continuity equation

$$u_c = \frac{\dot{m}}{\rho_c A_c}$$

using the correct area (A_c) and ρ_c from Eq. (51).

4.6 COMPUTATION OF AREA

The flow area (A) is required as a function of x in an integration interval. This function need not be specified as a function of distance from the origin; thus, any complex geometrical configuration can be handled readily with a simple function for the integration interval only.

Let

$$A_c = A_o e^{\beta \Delta x} \quad (52)$$

where A_c is the area at the end of an interval, and A_o is the area at the beginning of an interval

$$\therefore \beta = \frac{1}{\Delta x} \ln \left(\frac{A_c}{A_o} \right) \quad (53)$$

Equations (52) and (55) are to be used in Eqs. (42), (43), (44), and (47)

1. If the area is constant throughout: $\beta = 0$.
2. If the pressure is constant throughout: $\beta = -\delta$ (from the continuity equation).
3. If the pressure is specified as a function of distance from the origin, then the momentum equation and differential form of the energy equation

$$\frac{dH}{dx} = -u \frac{du}{dx} = + \frac{1}{\rho} \frac{dp}{dx} \quad (54)$$

is solved for H_c , u_c , and p_c and the area can be obtained from the continuity equation:

$$A_c = A_o e^{\beta \Delta x} = \frac{\dot{m}}{\rho_c u_c} \quad (55)$$

$$\therefore \beta = \frac{1}{A_o} \ln \left[\frac{\dot{m}}{u_o \rho_c u_c} \right] \quad (56)$$

4.7 STEPSIZE CONTROL AND INITIAL STEPSIZE

An effective stepsize control is presented based on the error generated in the solution of the linearized algebraic equations. This is accomplished by a comparison of the results obtained from the two concentration derivatives (Eqs. (40) and (41)) integrated in the residual Eq. (42).

$$(\gamma_i)_X - \Delta X = (\gamma_i)_X + \Delta \gamma_i$$

$$\Delta \gamma_i \approx \frac{d\gamma_i}{dX} \cdot \Delta X$$

$$\text{Equation 40: } (\Delta \gamma_i)_1 = \frac{1}{\rho} (d_{i1} + 2d_{i2} \Delta X - \delta \gamma_i) \quad i = 1, n_A$$

$$\text{Equation 41: } (\Delta \gamma_i)_2 = \left(\frac{\dot{m}}{A} \right)^{-1} \sum_{k=1}^n a_{ik} \gamma_k - c_i \quad i = 1, n_A$$

At each integration step a comparison is made of the above calculations and a check for significance of the error is also included

$$\frac{|(\Delta \gamma_i)_2 - (\Delta \gamma_i)_1|}{(\gamma_i)_X + \Delta X} \leq \text{significant figure in the value of } (\gamma_k)_X + \Delta X$$

SECTION V NUMERICAL CALCULATIONS AND RESULTS

Method 3 has been programmed and found to be a very effective method of analyzing one-dimensional (or streamtube) nonequilibrium flows. The calculated results are at least as accurate as those obtained by classical methods, and computation time can be reduced drastically in the cases where classical methods are very time consuming.

5.1 EXAMPLE OF CONSTANT PRESSURE COMBUSTION

This example involves a long ignition delay, followed by a short period of heat release, followed by a long period of near-equilibrium

flow. A Runge-Kutta, predictor-corrector calculation (Ref. 9) was carried out for a duct 450 cm long having an initial static temperature of 1111°K and an initial static pressure of 0.5 atm in 2 hr 59 min of computer time on an IBM 360/50. The results are shown in Figs. 1a through e, Appendix I. The present method was used with several values of stepsize control criteria: 0.0005; 0.005; and 0.05. No significant difference occurred between the Runge-Kutta, predictor-corrector results and the present method except for the largest value of stepsize control criteria (0.05) where differences of a few percent were obtained during the period of fast heat release. Computation time was:

29 min 35 sec at 0.0005 stepsize control criteria

13 min 31 sec at 0.005 stepsize control criteria

11 min 43 sec at 0.05 stepsize control criteria.

The savings in computation time were appreciable. The differences of a few percent obtained in the 0.05 control case are somewhat nebulous since the reaction rate data are not known sufficiently accurately to determine quantitative data to this accuracy.

5.2 EXAMPLE OF CONSTANT AREA COMBUSTION

This example involves a short ignition delay followed by a period of fast reaction. A Runge-Kutta, predictor-corrector calculation was carried out in 3 min 47 sec for a duct 12.7 cm long having an initial static temperature of 1160°K and an initial static pressure of 1.861 atm. The results are shown in Figs. 2a through f. The present method was used with the same stepsize control criteria with no significant differences in calculated results. Computation time was:

3 min 48 sec at 0.005 stepsize control criteria

1 min 59 sec at 0.05 stepsize control criteria.

Again, significant savings in computation time were obtained. This particular case is favorable to the Runge-Kutta predictor-corrector method because the periods in which the equations are stiff are short (ignition delay and approaching equilibrium). Further savings in computation time are obtained if certain terms in the linearized coefficients ($a_{i,k}$) are separated. Only a small fraction of the $a_{i,k}$ terms involve the parameters δ and β , and these terms only need be calculated at each iteration.

5.3 EXAMPLE OF EXPANDING STREAMTUBE FLOW

5.3.1 Specified Area

This type of calculation is difficult to carry out for two reasons:

1. Species production equations tend to "freeze" as the density and temperature decrease.
2. The approximate Eq. (30) is no longer a linear equation with constant coefficients since $\left(\frac{\dot{m}}{A}\right)^{-1}$ is a function of streamtube distance.

Condition (1) tends to make the determinant of the species coefficient matrix tend to zero; hence, the accuracy in the inversion of the matrix becomes progressively poor. The result of errors caused by condition (1) and particularly condition (2) appears as an oscillation in the values of computed variables. The amplitude of the oscillation is controlled by the stepsize control criteria. It is quite small for 0.005 as shown in Figs. 3a and b. The geometry is shown in Fig. 3c, consisting of a parabolic turning section which matches the slopes of the constant area combustor and a 15-deg conical expansion section. The oscillation is, of course, removed by setting the rate Eqs. (40) and (41) equal to zero when the contribution to the fluid-dynamic equations is reduced to a negligible amount (flow is effectively frozen).

5.3.2 Specified Pressure as a Function of x

The integration of the momentum and energy equations involves no additional errors (the area equation (Eq. (52)) is not used) and no oscillation is obtained. This calculation proceeds much faster than the above specified area case.

Since the specified pressure cases generate inherently more accurate calculations, it is preferable to evaluate one calculation for specified area and use the calculated pressure distribution as an initially specified function of x for additional calculations. This is also suggested for the additional reason that specified area distribution cases ignore wall boundary layers.

5.4 FROZEN FLOW

This calculation required about 20 sec of computing time for the geometry of Fig. 3c. The species rate Eqs. (40) and (41) are set equal

to zero and the momentum equation is integrated directly as it is a function of the assumed density change and given area variation only. The energy equation is solved as before to obtain a temperature which is compared with the value from the equation of state. An upper limit on stepsize is necessary to ensure smooth plots. A temperature and pressure profile is shown in Figs. 4a and b (data correspond to Section III).

5.5 EXAMPLE OF INFLUENCE OF INITIAL CONCENTRATIONS

The Runge-Kutta predictor-corrector program used to establish computer time for comparison purposes employed atomic conservation equations for the concentrations of hydrogen and oxygen atoms. Thus initial values of these concentrations can never be zero since round-off error in the initial values of hydrogen and oxygen molecules generates initial values of the corresponding atom concentrations. For this reason the initial values generated by the Runge-Kutta predictor-corrector program were used as initial values for the present program and are shown below (mass fractions are actual input values):

<u>i</u>	<u>γ_i</u>	<u>moles/gm</u>	
1	(H)	$= 1.25992 \times 10^{-8}$	Density (ρ) $= 5.28314 \times 10^{-4}$ gm/cm ³
2	(O)	$= 1.96875 \times 10^{-10}$	Pressure (p) $= 1.861$ atm
3	(H ₂ O)	$= 5.55062 \times 10^{-18}$	Temperature (T) $= 1159.6^\circ\text{K}$
4	(OH)	$= 5.87959 \times 10^{-18}$	Velocity (u) $= 1.4129 \times 10^5$ cm/sec
5	(O ₂)	$= 6.86381 \times 10^{-3}$	$= 4635.5$ ft/sec
6	(H ₂)	$= 2.48016 \times 10^{-3}$	
7	(N ₂)	$= 2.76755 \times 10^{-2}$	

The results of computations with these values were discussed earlier and are given in Figs. 2a through d.

These initial values for hydrogen and oxygen atom concentrations completely swamp the effect of including reaction 1 as suggested in Ref. 10. This is readily illustrated with the present program by computing the results with these two concentrations set equal to some negligible number (mass fractions of 10^{-16} were used) and setting reaction rate $f_1 = 0$. These results are shown in Figs. 5a and b. If the initial

concentrations are maintained at this negligible quantity and reaction rate f_1 is included, the results are again similar to Figs. 2a and b as shown in Figs. 5c and d. Reaction 1 is an initiation mechanism which is necessary to describe the process by which the chain reaction ignition reactions can start.

These results point out the usefulness of being able to set the initial concentrations of any species at any desired value. This capability is absolutely essential for studies of ignition delay or vitiation.

SECTION VI NORMAL SHOCK CALCULATIONS

The composition of the streamtube flow is assumed to be frozen just upstream of the normal shock. The values of fluid-dynamic and state variables behind the normal shock are obtained by an iterative solution to the conservation equations (Eqs. (10), and (12)), and the equation of state (Eq. (15)). These computed values together with the assumed frozen composition are restored to the nonequilibrium program as initial values and the approach to equilibrium behind the normal shock is then calculated. A normal shock at any station in the combustor or nozzle can be evaluated.

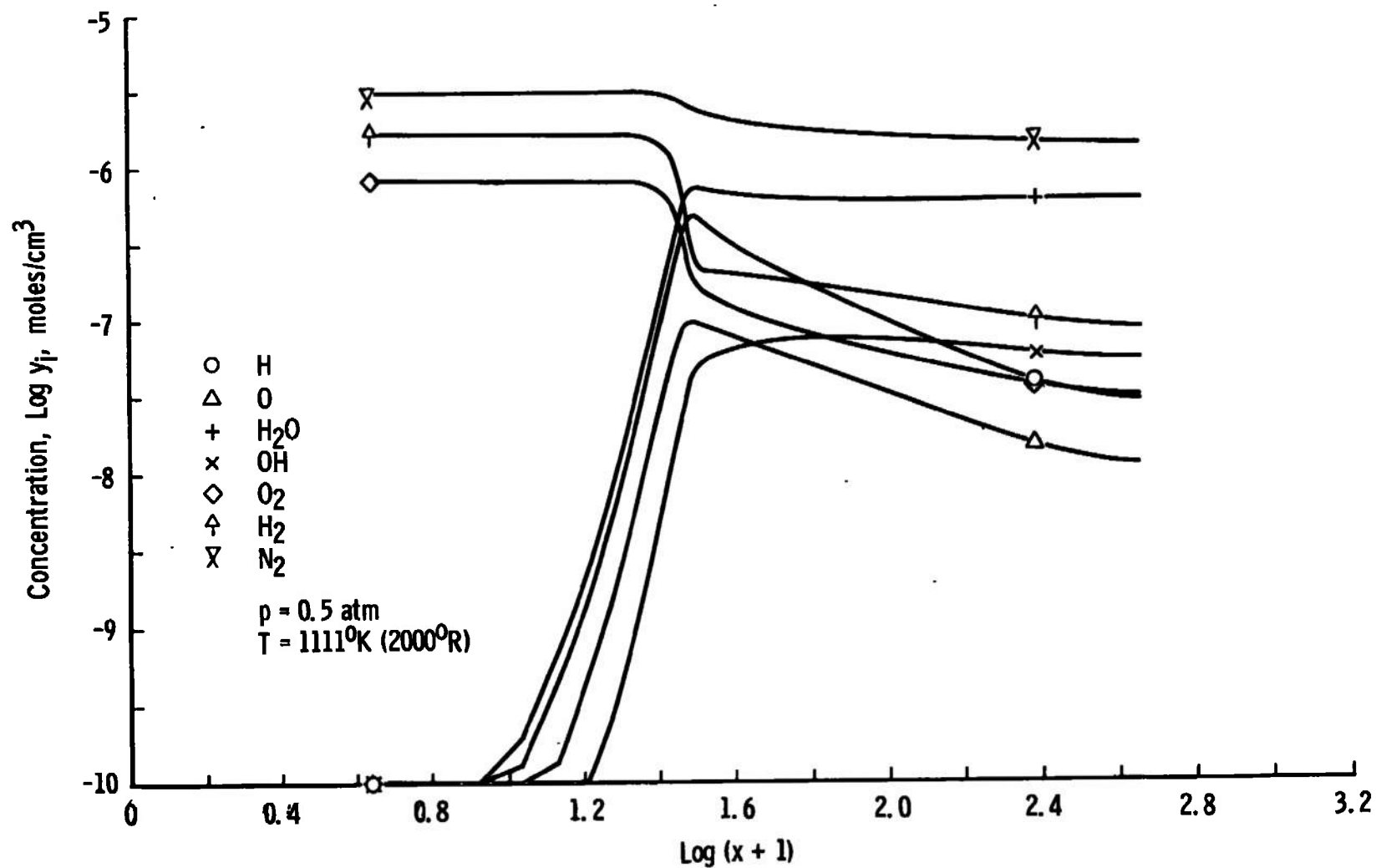
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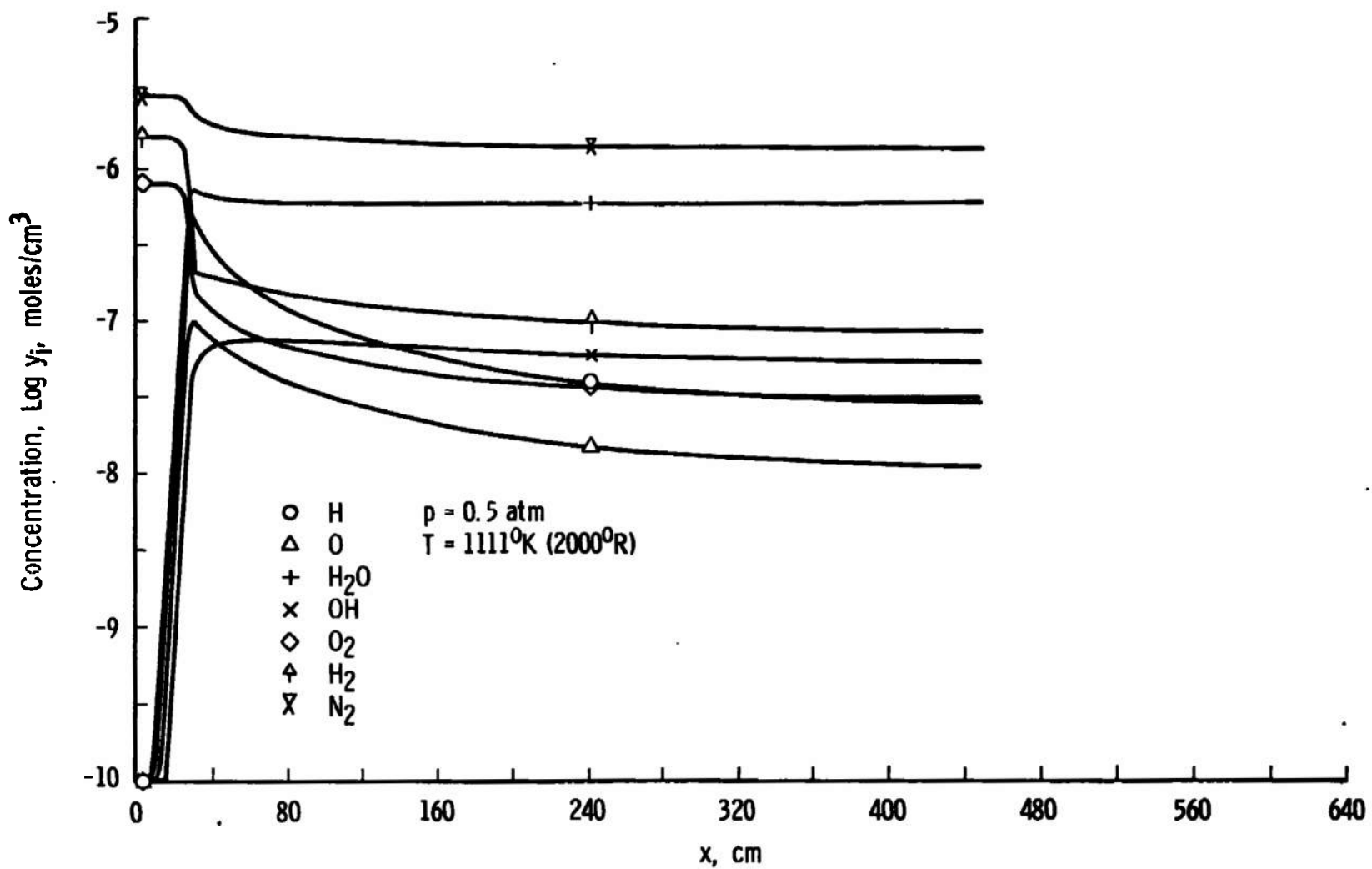
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APPENDIXES

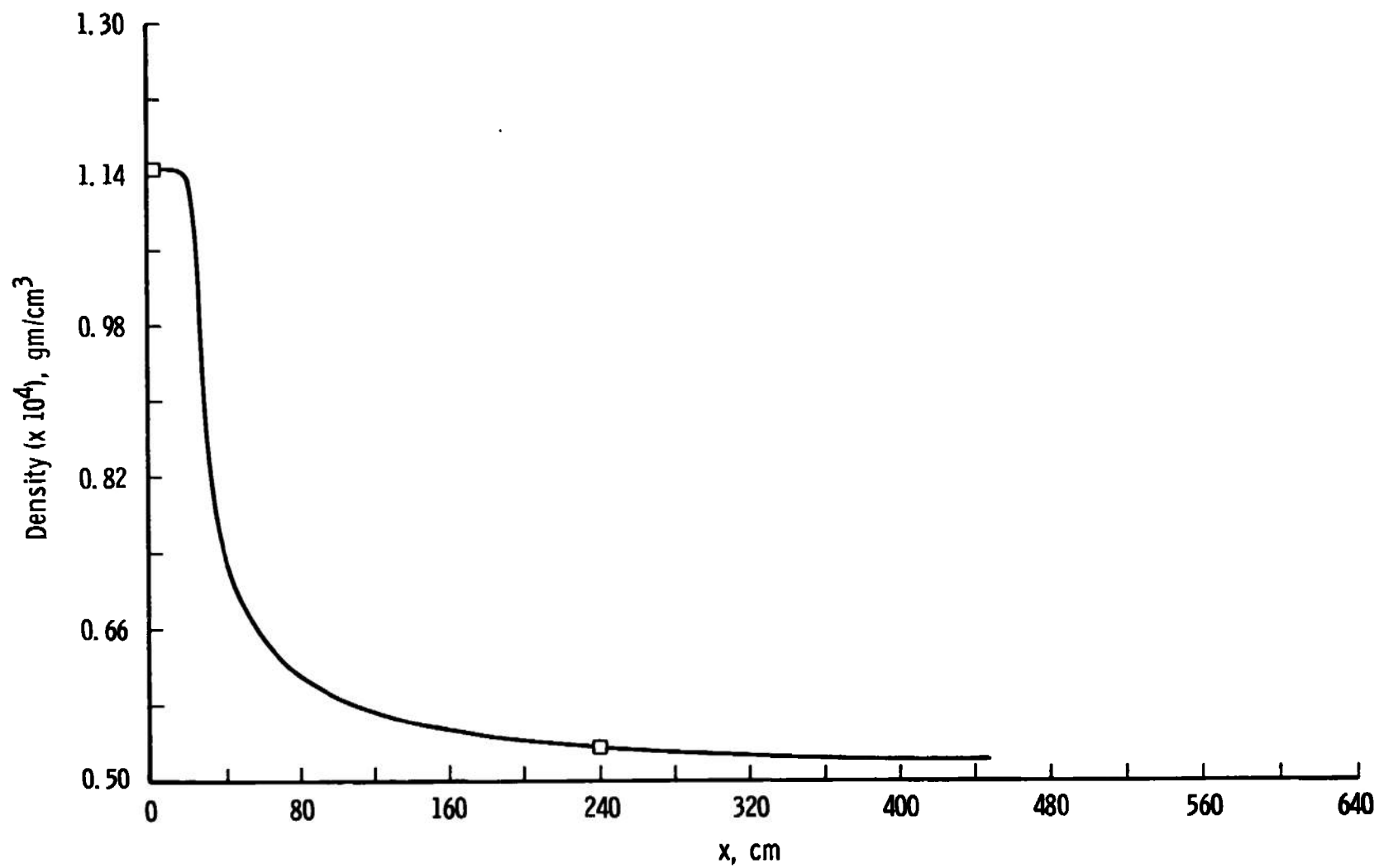
- I. ILLUSTRATIONS**
- II. REACTION RATE COEFFICIENTS**
- III. ENTHALPY FIT COEFFICIENTS**
- IV. LINEARIZED COEFFICIENTS**



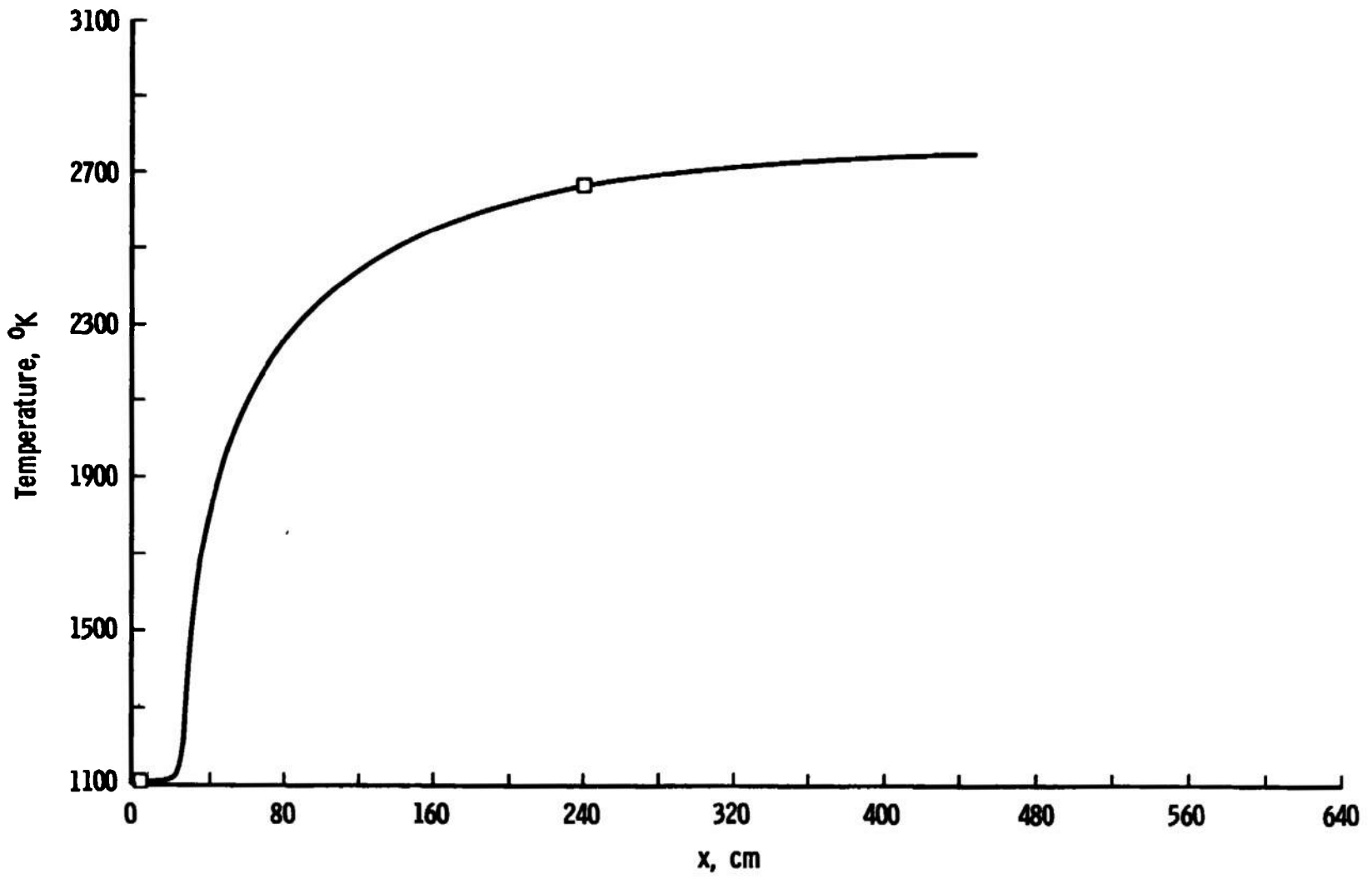
a. Concentration Profiles
 Fig. 1 Constant Pressure Combustion



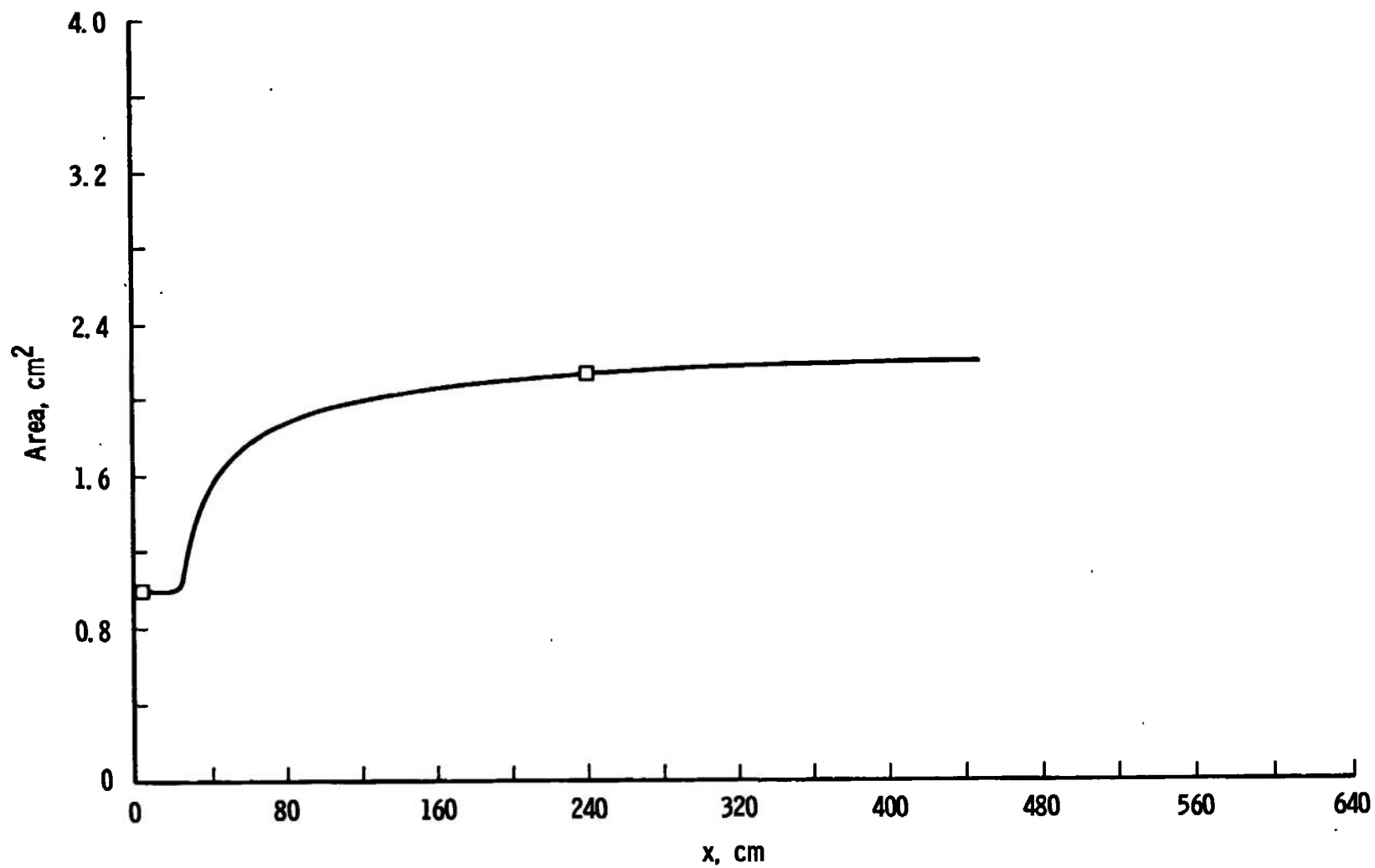
b. Concentration Profiles
 Fig. 1 Continued



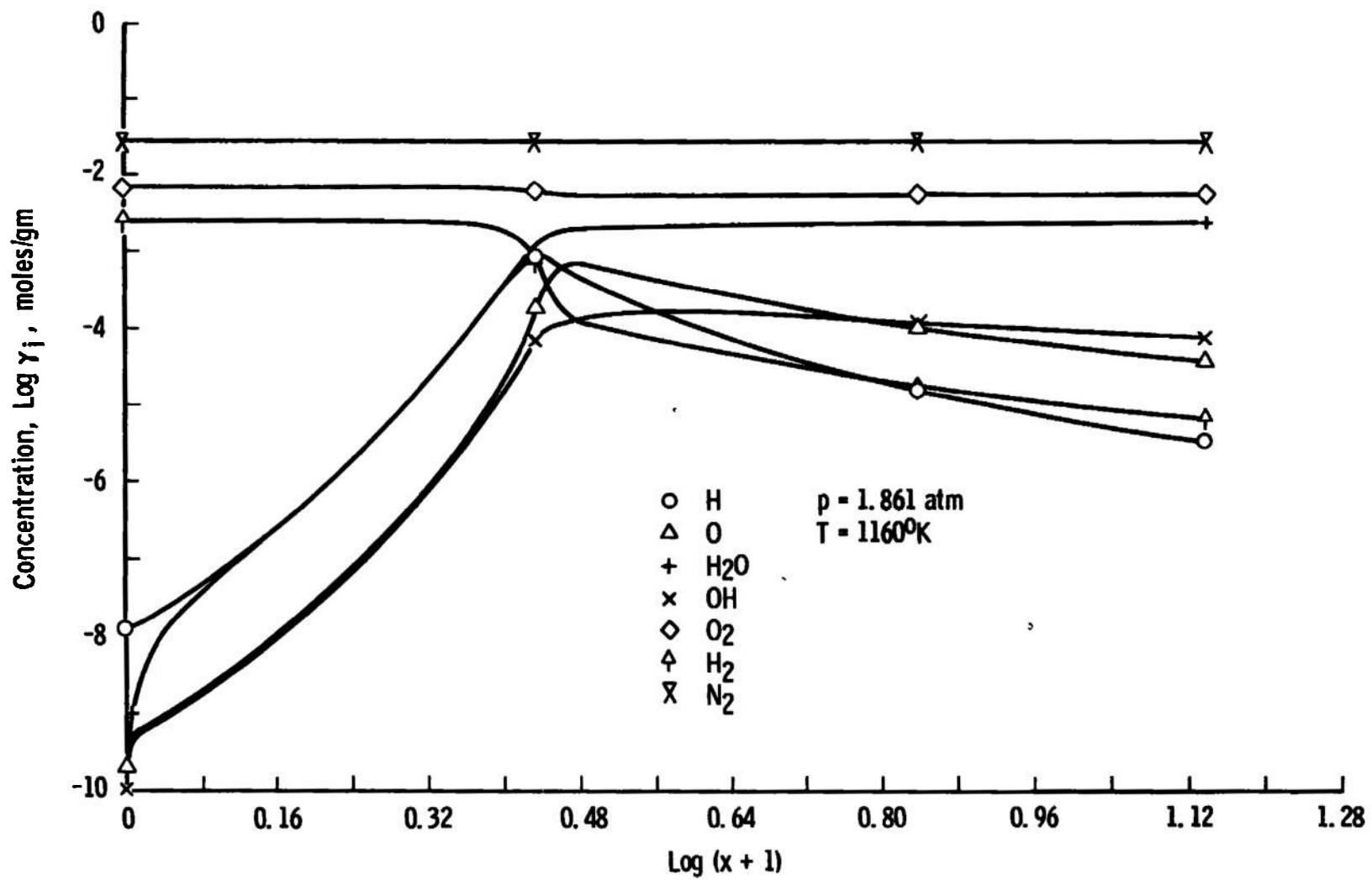
c. Density Profile
Fig. 1 Continued



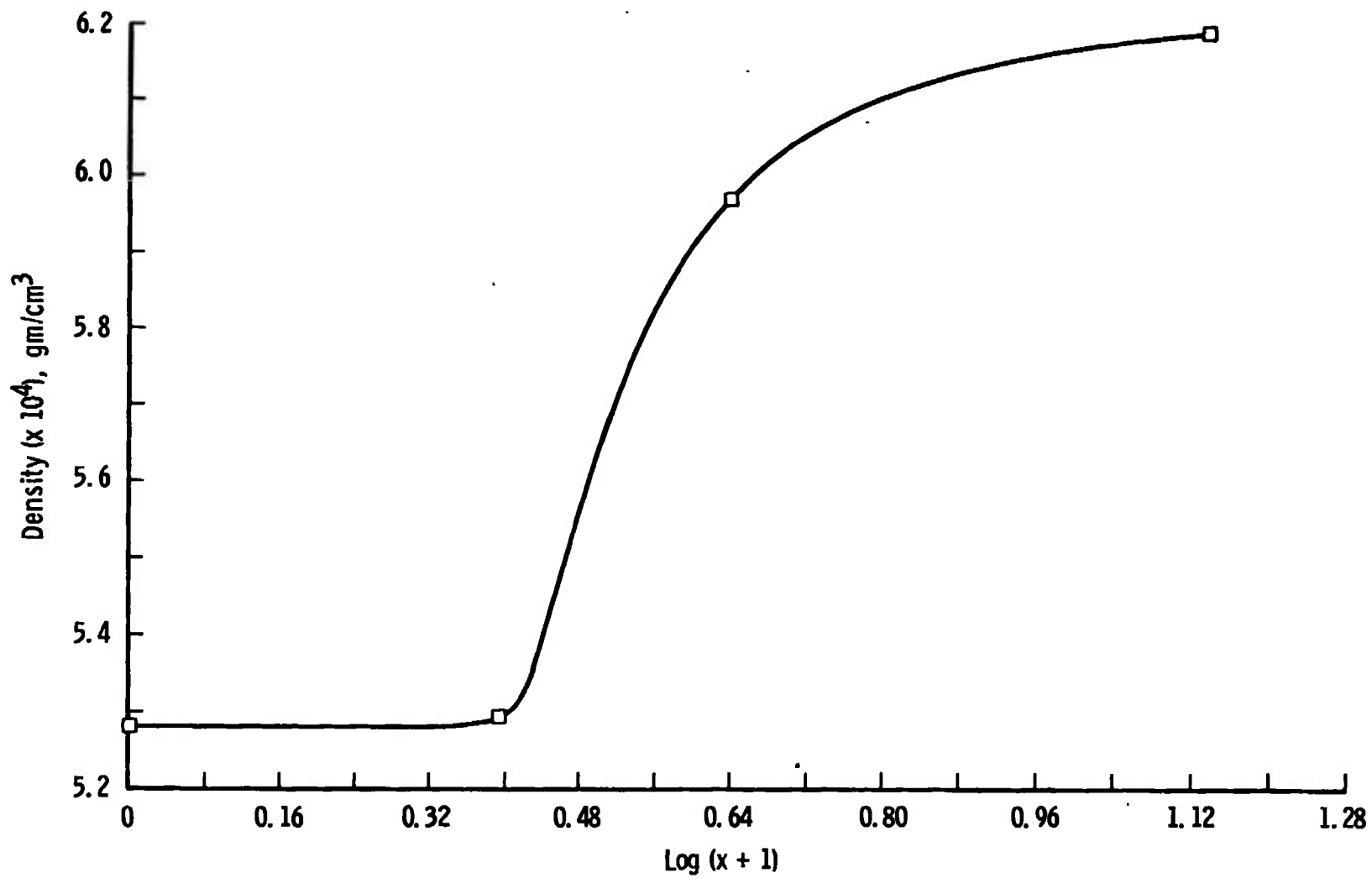
d. Temperature Profile
Fig. 1 Continued



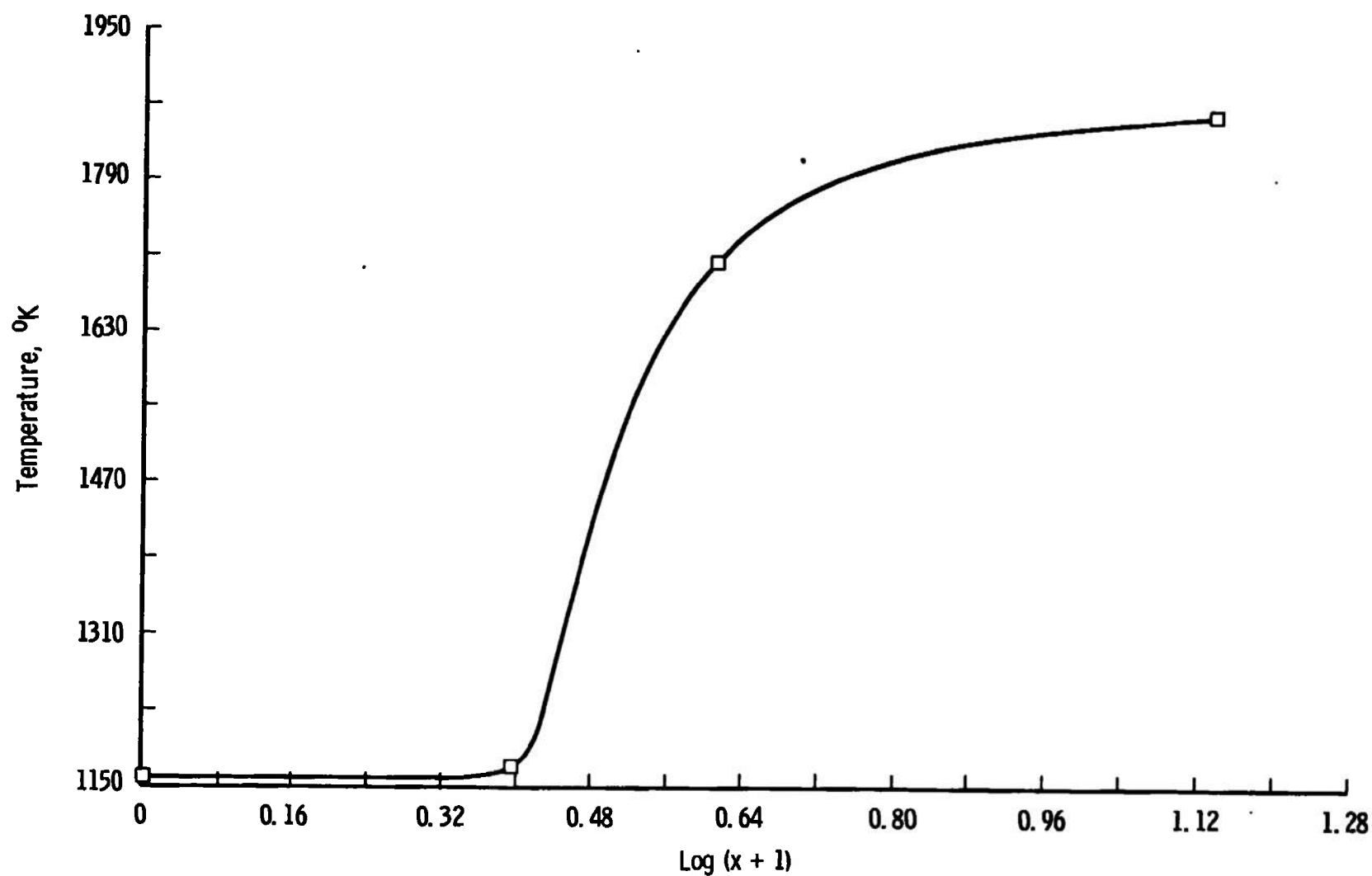
e. Streamtube Area
Fig. 1 Concluded



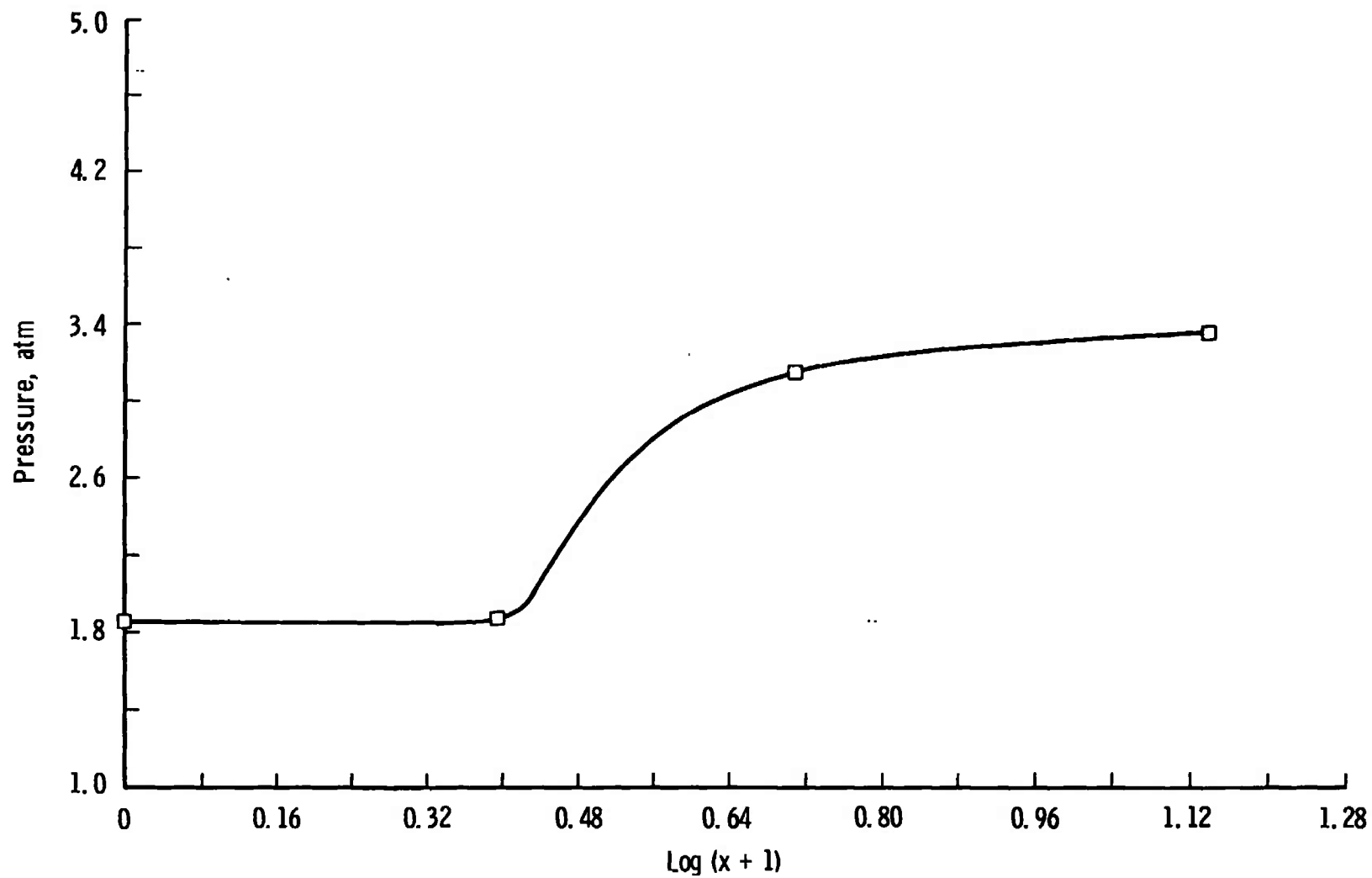
a. Concentration Profiles
 Fig. 2 Constant Area Combustion



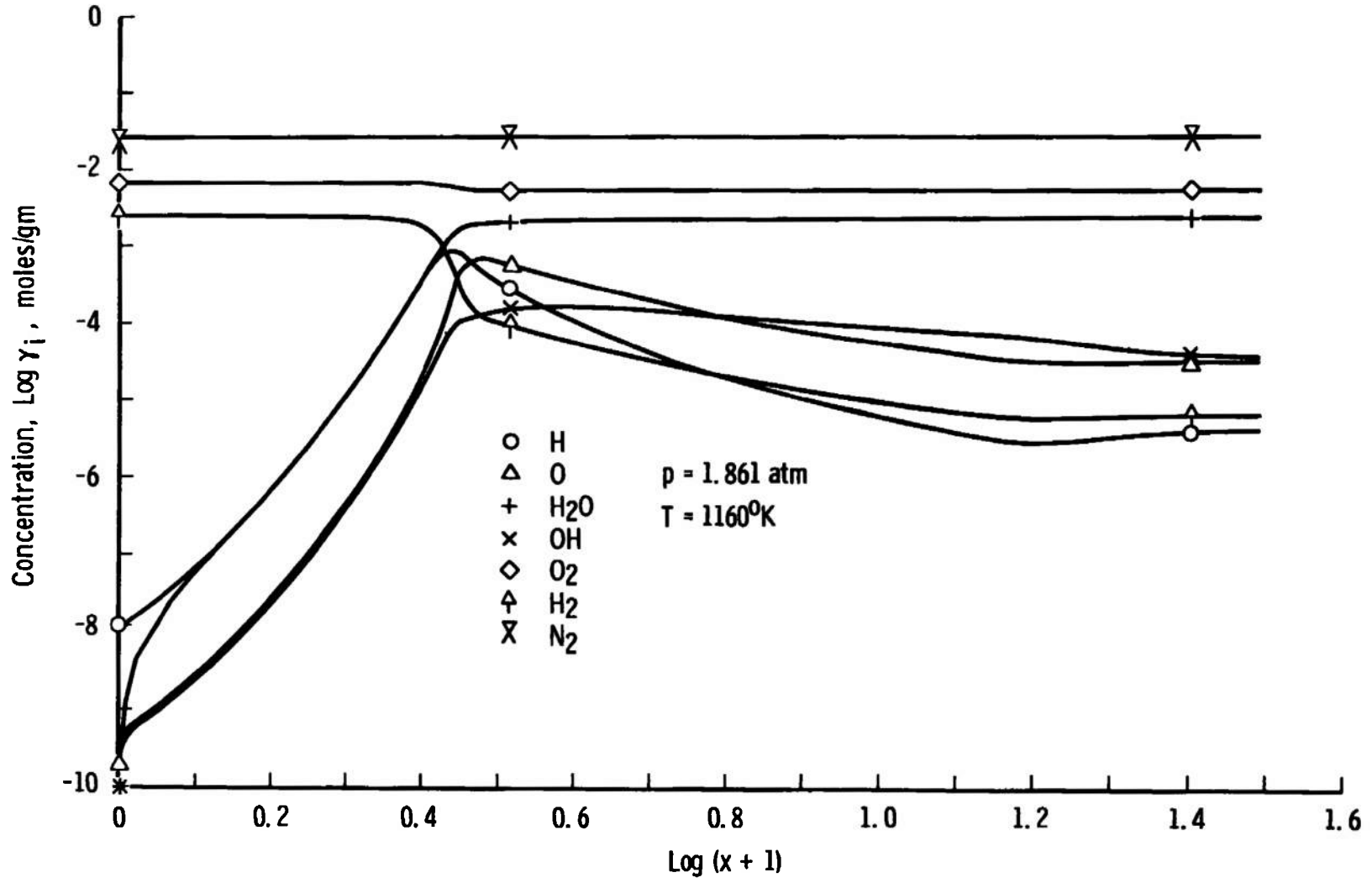
b. Density Profile
Fig. 2 Continued



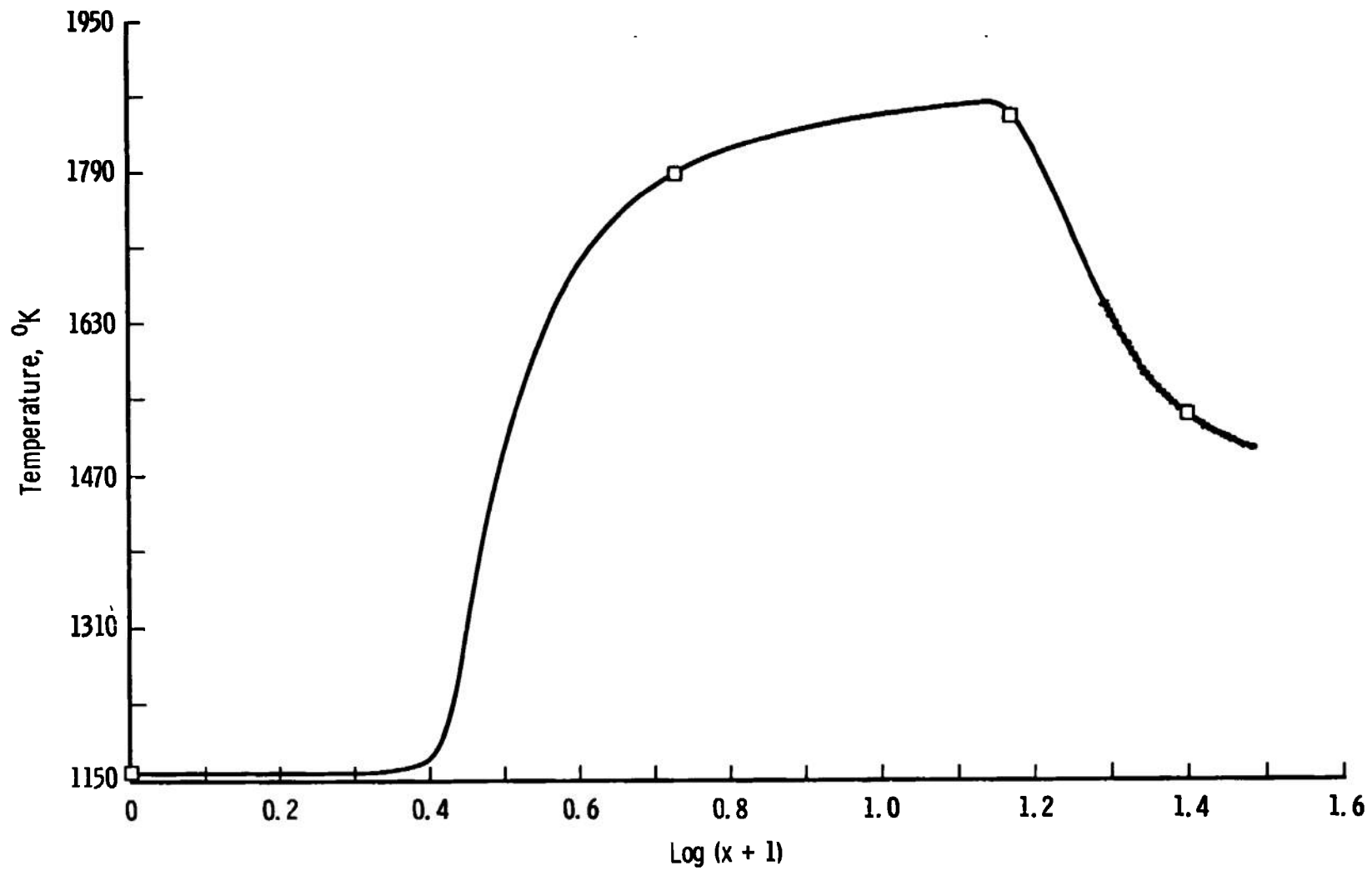
c. Temperature Profile
Fig. 2 Continued



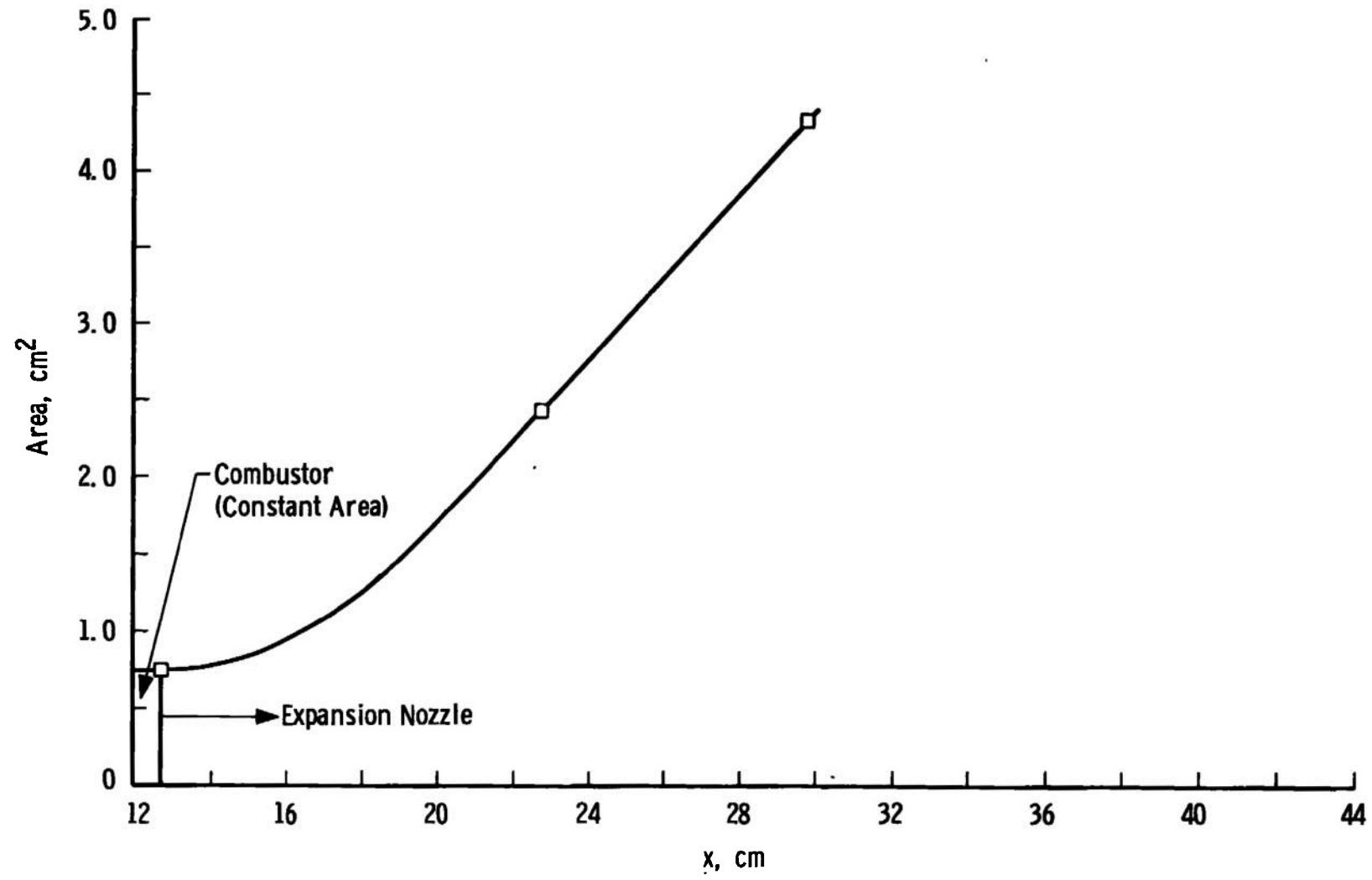
d. Pressure Profile
Fig. 2 Concluded



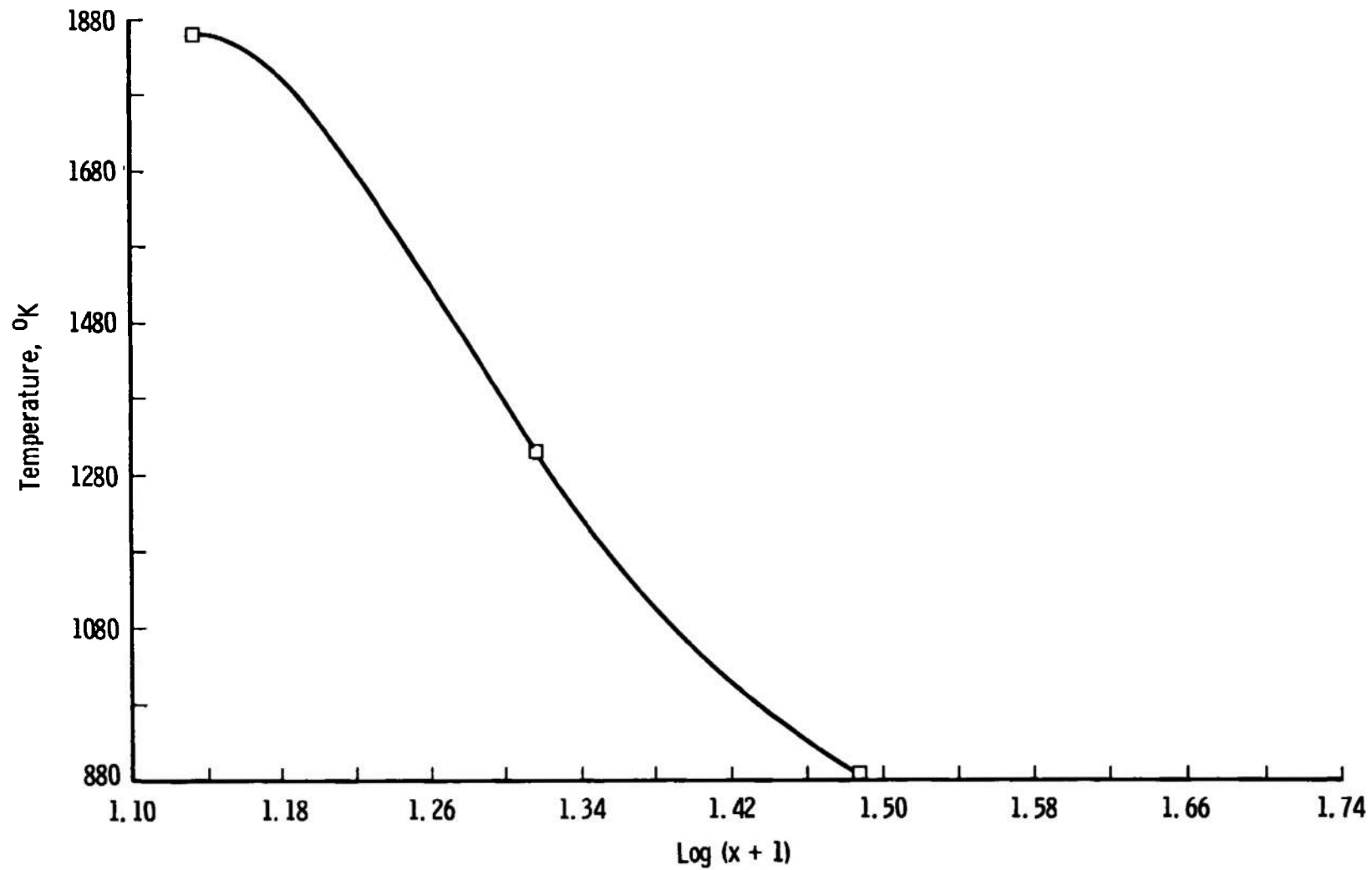
a. Concentration Profile
 Fig. 3 Expanding Nozzle Flow



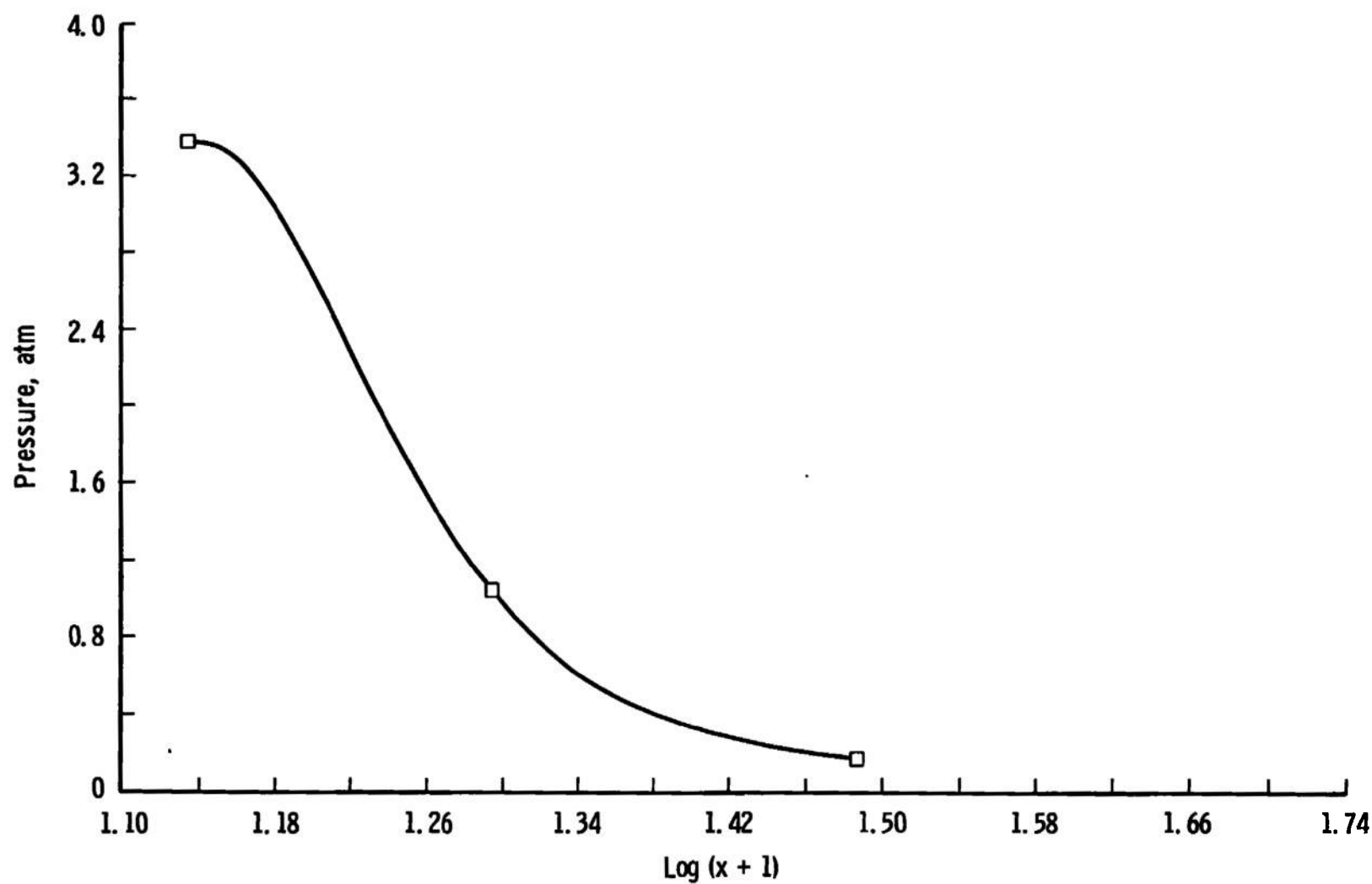
b. Temperature Profile
Fig. 3 Continued



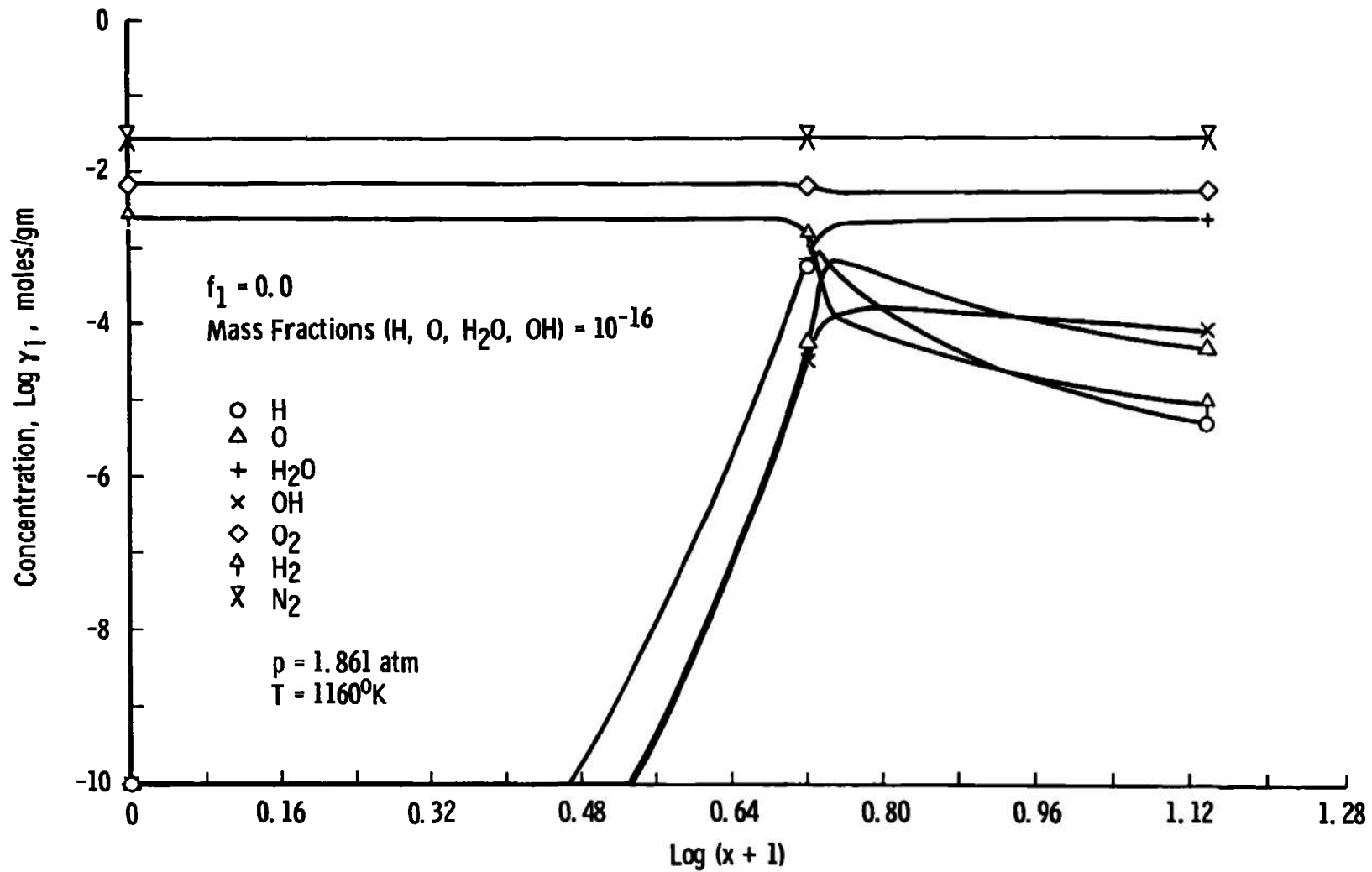
c. Nozzle Geometry
Fig. 3 Concluded



a. Temperature Profile
Fig. 4 Frozen Nozzle Flow

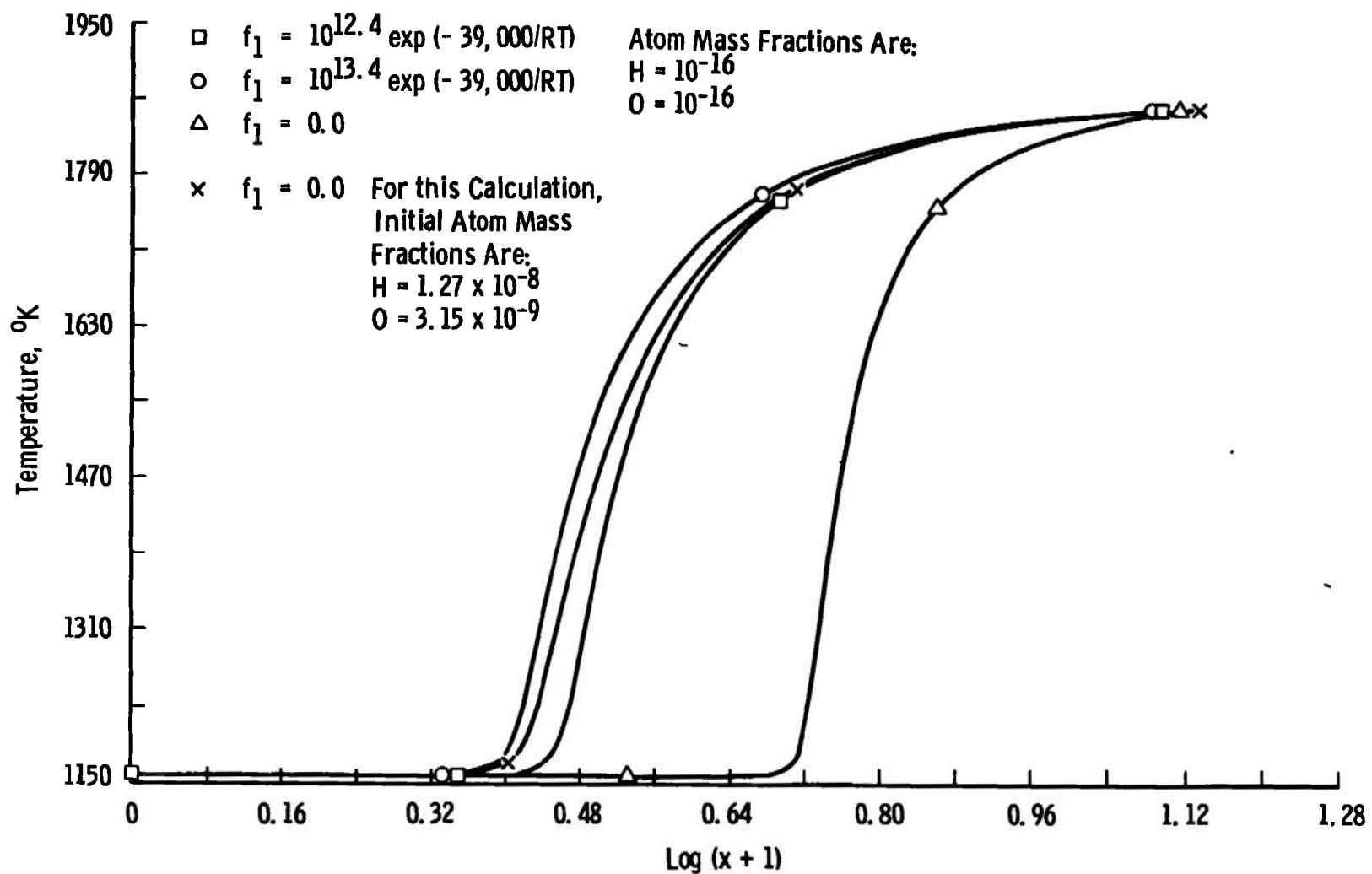


b. Pressure Profile
Fig. 4 Concluded

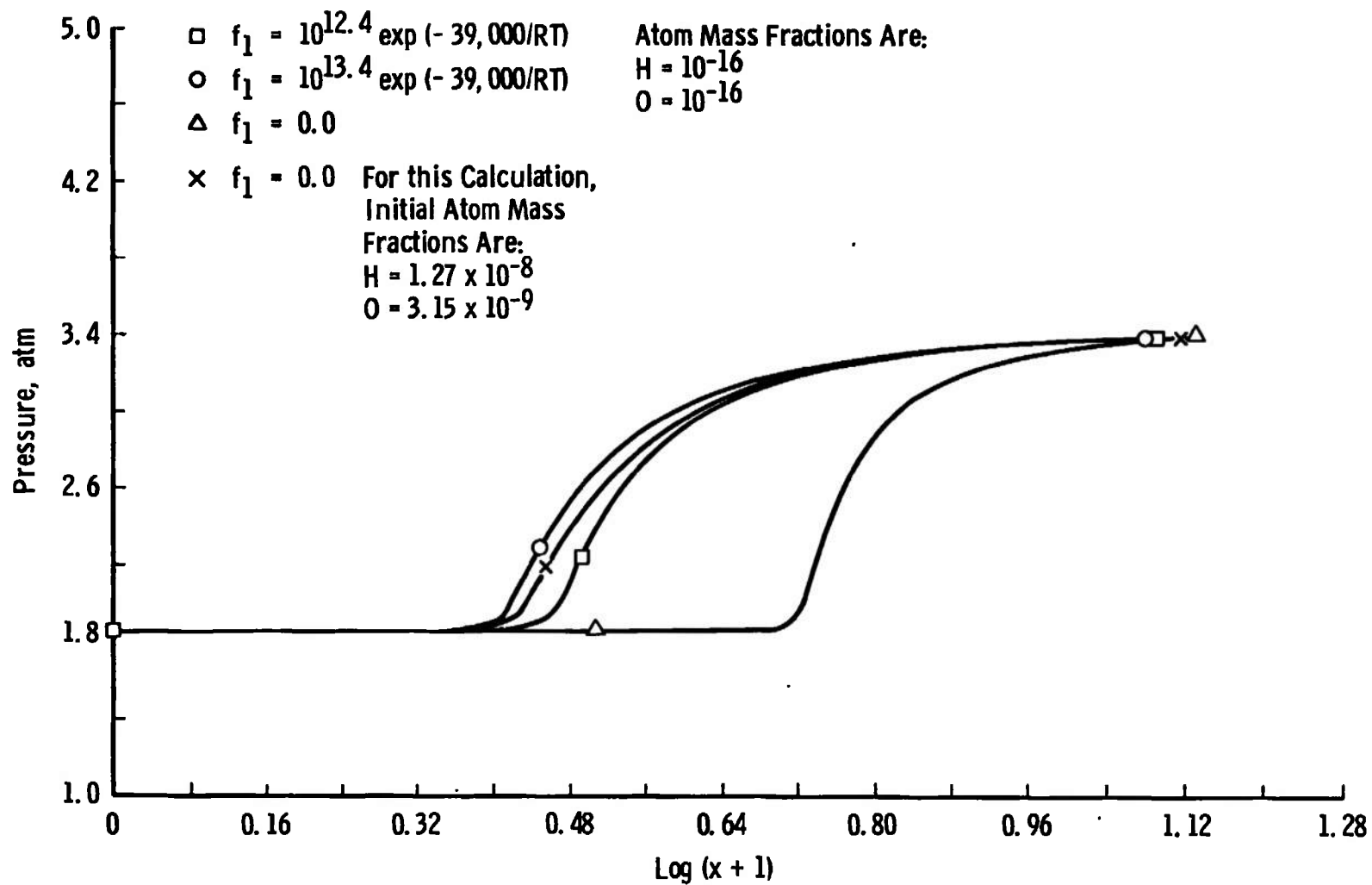


a. Concentration Profiles

Fig. 5 Constant Area Combustion (Influence of Initial Conditions)



b. Temperature Profiles
 Fig. 5 Continued



c. Pressure Profiles
 Fig. 5 Concluded

APPENDIX II
REACTION RATE COEFFICIENTS

<u>j</u>	<u>f_j</u>	<u>Units</u>	<u>b_j</u>	<u>Ref.</u>
1	$1.0 \times 10^{12.4} e^{-19.625/\bar{T}}$	$\text{cm}^3/\text{mole sec}$	0	10
2	$3 \times 10^{14} e^{-8.81/\bar{T}}$	↓	$2.48 \times 10^{13} e^{-0.66/\bar{T}}$	5
3	$3 \times 10^{14} e^{-4.03/\bar{T}}$		$1.3 \times 10^{14} e^{-2.49/\bar{T}}$	↓
4	$3 \times 10^{14} e^{-3.02/\bar{T}}$		$1.33 \times 10^{15} e^{-10.95/\bar{T}}$	
5	$3 \times 10^{14} e^{-3.02/\bar{T}}$		$3.12 \times 10^{15} e^{-12.51/\bar{T}}$	
6	$1.85 \times 10^{17} T^{-1} e^{-54/\bar{T}}$		10^{16}	
7	$9.66 \times 10^{18} T^{-1} e^{-62.2/\bar{T}}$	↓	10^{17}	↓
8	$8 \times 10^{16} T^{-1} e^{-52.2/\bar{T}}$		10^{16}	
9	$5.8 \times 10^{16} T^{-1} e^{-60.6/\bar{T}}$		6×10^{14}	

where

$$\bar{T} = T/1000.$$

APPENDIX III ENTHALPY FIT COEFFICIENTS

The partial enthalpies (in K cal/gm) are fitted by means of the following equations (Ref. 5, based on curve fitted data from Ref. 8):

$$h_i = \begin{cases} A_i + B_i \bar{T} & \bar{T} \leq \bar{T}_{oi} \\ A_i + B_i \bar{T} + C_i(\bar{T} - \bar{T}_{oi})^2 & \bar{T}_{oi} \leq \bar{T} \leq \bar{T}_{li} \\ D_i + E_i \bar{T} & \bar{T}_{li} \leq \bar{T} \leq 6 \end{cases}$$

$$\bar{T} = \frac{T}{10^3} \text{ } ^\circ\text{K}$$

i	A _i	B _i	C _i	D _i	E _i	\bar{T}_{oi}	\bar{T}_{li}
1	50.22	4.93	0.0	0.0	0.0	6.0	6.0
2	3.622	0.3187	0.0	0.0	0.0	6.0	6.0
3	-3.3395	0.4464	0.0681	-3.9456	0.7902	0.5	3.94
4	0.4247	0.4158	0.0201	0.1631	0.5422	0.5	3.64
5	-0.0648	0.2206	0.0198	-0.2297	0.3168	0.5	2.93
6	-1.004	3.403	0.1968	-4.286	4.831	0.5	4.096
7	-0.074	0.2488	0.019	-0.1859	0.3239	0.5	2.48

Coefficients in Eqs. (48) and (49) are:

$$A^* = \sum_{i=1}^{nT} \alpha_i C_i \quad B^* = \sum_{i=1}^{nT} \alpha_i (C_i T_{oi} - B_i/2) \quad C^* = \sum_{i=1}^{nT} \alpha_i (A_i + C_i T_{oi}^2)$$

APPENDIX IV LINEARIZED COEFFICIENTS

From Eq. (3)

$$\dot{y}_i = \sum_{j=1}^9 \dot{y}_{ij} \quad (\text{IV-1})$$

From Eq. (9)

$$\frac{dy_i}{dx} = \frac{1}{\rho u} \dot{y}_i = \left(\frac{\dot{m}}{A}\right)^{-1} \dot{y}_i \quad (\text{IV-2})$$

$$= \left(\frac{\dot{m}}{A}\right)^{-1} \left[\sum_{k=1}^4 a_{ik} y_k + c_i \right] \quad (\text{IV-3})$$

Using Taylor series expansion of the right-hand side of Eq. (IV-1):

$$\dot{y}_{ij} = \dot{y}_{ij}^0 + \sum_{k=1}^4 \frac{\partial \dot{y}_{ij}^0}{\partial y_k} \{y_k - y_k^0\} \quad (\text{IV-4})$$

where ()⁰ means evaluate at the beginning of an integration interval.

Equation IV-1 becomes

$$\dot{y}_i = \sum_{j=1}^9 \dot{y}_{ij}^0 + \sum_{k=1}^4 \sum_{j=1}^9 \frac{\partial \dot{y}_{ij}^0}{\partial y_k} \{y_k - y_k^0\} \quad (\text{IV-5})$$

$$= \sum_{k=1}^4 \sum_{j=1}^9 \frac{\partial \dot{y}_{ij}^0}{\partial y_k} y_k + \sum_{j=1}^9 \left[\dot{y}_{ij}^0 - \sum_{k=1}^4 \frac{\partial \dot{y}_{ij}^0}{\partial y_k} y_k^0 \right] \quad (\text{IV-6})$$

$$= \sum_{k=1}^4 a_{ik} y_k + c_i \quad (\text{IV-7})$$

$$\therefore a_{ik} = \sum_{j=1}^9 \frac{\partial \dot{y}_{ij}^0}{\partial y_k} \quad (\text{IV-8})$$

and

$$c_i = \sum_{j=1}^9 \left[\dot{y}_{ij}^0 - \sum_{k=1}^4 \frac{\partial \dot{y}_{ij}^0}{\partial y_k} y_k^0 \right] \quad (\text{IV-9})$$

The \dot{y}_{ij} are tabulated as follows:

$$\begin{array}{llll}
 \dot{y}_{11} = 0 & \dot{y}_{21} = 0 & \dot{y}_{31} = 0 & \dot{y}_{41} = \dot{y}_{41} \\
 \dot{y}_{12} = -\dot{y}_{22} & \dot{y}_{22} = \dot{y}_{22} & \dot{y}_{32} = 0 & \dot{y}_{42} = \dot{y}_{22} \\
 \dot{y}_{13} = \dot{y}_{13} & \dot{y}_{23} = -\dot{y}_{13} & \dot{y}_{33} = 0 & \dot{y}_{43} = \dot{y}_{13} \\
 \dot{y}_{14} = \dot{y}_{14} & \dot{y}_{24} = 0 & \dot{y}_{34} = \dot{y}_{14} & \dot{y}_{44} = -\dot{y}_{14} \\
 \dot{y}_{15} = 0 & \dot{y}_{25} = \dot{y}_{23} & \dot{y}_{35} = \dot{y}_{23} & \dot{y}_{45} = -2\dot{y}_{23} \\
 \dot{y}_{16} = \dot{y}_{16} & \dot{y}_{26} = 0 & \dot{y}_{36} = 0 & \dot{y}_{46} = 0 \\
 \dot{y}_{17} = \dot{y}_{17} & \dot{y}_{27} = 0 & \dot{y}_{37} = -\dot{y}_{17} & \dot{y}_{47} = \dot{y}_{17} \\
 \dot{y}_{18} = \dot{y}_{18} & \dot{y}_{28} = \dot{y}_{18} & \dot{y}_{38} = 0 & \dot{y}_{48} = -\dot{y}_{18} \\
 \dot{y}_{19} = 0 & \dot{y}_{29} = \dot{y}_{29} & \dot{y}_{39} = 0 & \dot{y}_{49} = 0
 \end{array} \tag{IV-10}$$

where $i = 1, 2, 3$, and 4 are the only species considered since y_5 and y_6 are given by Eq. (25) and nitrogen is inert.

Only nine of the terms in Eqs. IV-10 are to be determined since the remaining terms are either zero or differ by some integer which can be positive or negative. The following form can thus be used:

$$\dot{y}_{ij} = \sum_{k=1}^4 \sum_{j=1}^9 S_{ij} R_{kj} y_k + \sum_{j=1}^9 \left[S_{ij} R_{ij}^o - \sum_{k=1}^4 S_{ij} R_{kj} y_k^o \right] \tag{IV-11}$$

where

$$a_{ik} = \sum_{j=1}^9 S_{ij} R_{kj} \tag{IV-12}$$

$$c_i = \sum_{j=1}^9 \left[S_{ij} R_{ij}^o - \sum_{k=1}^4 S_{ij} R_{kj}^o y_k^o \right] \tag{IV-13}$$

$$S_{ij} = \text{the integers in Eqs. (IV-10)} \tag{IV-14}$$

$$R_{ij}^o = \dot{y}_{ij}^o \tag{IV-15}$$

$$R_{kj} = \frac{\partial \dot{y}_{ij}^o}{\partial y_k} \tag{IV-16}$$

The R_{kj} are determined by differentiating Eqs. (5) after substitution of Eqs. (25):

$$\begin{aligned}
 y_5 &= b - 1/2 \{y_2 + y_3 + y_4\} \\
 y_6 &= c - 1/2 \{y_1 + 2y_3 + y_4\}
 \end{aligned} \tag{IV-17}$$

Substituting in Eqs. (5)

$$\begin{aligned}
 \dot{y}_{41} &= 2f_1 [b - 1/2 \{y_2 + y_3 + y_4\}] [c - 1/2 \{y_1 + 2y_3 + y_4\}] \\
 \dot{y}_{22} &= f_2 y_1 b - \frac{f_2}{2} y_1 \{y_2 + y_3 + y_4\} - b_2 y_2 y_4 \\
 \dot{y}_{13} &= f_3 y_2 c - \frac{f_3}{2} y_2 \{y_1 + 2y_3 + y_4\} - b_3 y_1 y_4 \\
 \dot{y}_{14} &= f_4 y_4 c - \frac{f_4}{2} y_4 \{y_1 + 2y_3 + y_4\} - b_4 y_1 y_3 \\
 \dot{y}_{25} &= f_5 y_4^2 - b_5 y_2 y_3 \\
 \dot{y}_{16} &= 2f_6 Y c - f_6 Y \{y_1 + 2y_3 + y_4\} - 2b_6 y_1^2 Y \\
 \dot{y}_{17} &= f_7 y_3 Y - b_7 y_1 y_4 Y \\
 \dot{y}_{18} &= f_8 y_4 Y - b_8 y_1 y_2 Y \\
 \dot{y}_{29} &= 2f_9 Y b - f_9 Y \{y_2 + y_3 + y_4\} - 2b_9 y_2^2 Y
 \end{aligned} \tag{IV-18}$$

Example:

$$\begin{aligned}
 \sum_{k=1} \frac{\partial \dot{y}_{22}}{\partial y_k} (y_k - y_k^0) &= f_2 [b - 1/2 \{y_2^0 + y_3^0 + y_4^0\}] (y_1 - y_1^0) - \left[\frac{f_2}{2} y_1^0 + b_2 y_4^0 \right] (y_2 - y_2^0) \\
 &\quad - \frac{f_2}{2} y_1^0 (y_3 - y_3^0) - \left[\frac{f_2}{2} y_1^0 + b_2 y_2^0 \right] (y_4 - y_4^0) \\
 &= R_{12}(y_1 - y_1^0) + R_{22}(y_2 - y_2^0) + R_{32}(y_3 - y_3^0) + R_{42}(y_4 - y_4^0)
 \end{aligned}$$

The coefficients R_{kj} are:

$k \backslash j$	1	2	3
1	$-f_1 \text{ Con } *$	$f_2 \text{ Con } *$	$-\left[\frac{f_3}{2} y_2^0 + b_3 y_4^0 \right]$
2	$-f_1 \text{ Com } *$	$-\left[\frac{f_2}{2} y_1^0 + b_2 y_4^0 \right]$	$f_3 \text{ Com } *$
3	$-f_1 (\text{Com} + 2\text{Con}) *$	$-\frac{f_2}{2} y_1^0$	$-f_3 y_2^0$
4	$-f_1 (\text{Com} + \text{Con}) *$	$-\left[\frac{f_2}{2} y_1^0 + b_2 y_2^0 \right]$	$-\left[\frac{f_3}{2} y_2^0 + b_3 y_1^0 \right]$

k \ j	4	5	6
1	$-\left[\frac{f_4}{2} y_4^{\circ} + b_4 y_3^{\circ}\right]$	0	$-\left[f_6 Y + 4b_6 y_1^{\circ} Y\right]$
2	0	$-b_5 y_3^{\circ}$	0
3	$-\left[f_4 y_4^{\circ} + b_4 y_1^{\circ}\right]$	$-b_5 y_2^{\circ}$	$-2f_6 Y$
4	$f_4 \left[\text{Com} - \frac{y_4^{\circ}}{2} \right]^*$	$2f_5 y_4^{\circ}$	$-f_6 Y$

k \ j	7	8	9
1	$-b_7 y_4^{\circ} Y$	$-b_8 y_2^{\circ} Y$	0
2	0	$-b_8 y_1^{\circ} Y$	$-\left[f_9 Y + 4b_9 y_2^{\circ} Y\right]$
3	$f_7 Y$	0	$-f_9 Y$
4	$-b_7 y_1^{\circ} Y$	$f_8 Y$	$-f_9 Y$

where

$$\text{Con} = b - 1/2 \{y_2^{\circ} + y_3^{\circ} + y_4^{\circ}\}$$

$$\text{Com} = c - 1/2 \{y_1^{\circ} + 2y_3^{\circ} + y_4^{\circ}\}$$

By inspection only seven terms involve δ , β through Con, Com and only these terms (marked *) need be evaluated at each iteration for δ .

The following coefficients are obtained from Eqs. (5):

$$R_{41}^{\circ} = 2f_1 y_5^{\circ} y_6^{\circ}$$

$$R_{22}^{\circ} = f_2 y_1^{\circ} y_5^{\circ} - b_2 y_2^{\circ} y_4^{\circ}$$

$$R_{13}^{\circ} = f_3 y_2^{\circ} y_6^{\circ} - b_3 y_1^{\circ} y_4^{\circ}$$

$$R_{14}^{\circ} = f_4 y_4^{\circ} y_6^{\circ} - b_4 y_1^{\circ} y_3^{\circ}$$

$$R_{25}^{\circ} = f_5 y_4^{\circ} y_6^{\circ} - b_5 y_2^{\circ} y_3^{\circ}$$

$$R_{16}^{\circ} = 2f_6 y_5^{\circ} Y - 2b_6 y_1^{\circ} Y$$

$$R_{17}^{\circ} = f_7 y_3^{\circ} Y - b_7 y_1^{\circ} y_4^{\circ} Y$$

$$R_{18}^{\circ} = f_8 y_4^{\circ} Y - b_8 y_1^{\circ} y_2^{\circ} Y$$

$$R_{29}^{\circ} = 2f_9 y_5^{\circ} Y - 2b_9 y_2^{\circ} Y$$

The coefficients R_{ij}° and S_{ij} are:

 R_{ij}°

$i \backslash j$	1	2	3	4	5	6	7	8	9
1	0	R_{22}°	R_{13}°	R_{14}°	0	R_{16}°	R_{17}°	R_{18}°	0
2	0	R_{22}°	R_{13}°	0	R_{25}°	0	0	R_{18}°	R_{29}°
3	0	0	0	R_{14}°	R_{25}°	0	R_{17}°	0	0
4	R_{41}°	R_{22}°	R_{13}°	R_{14}°	R_{25}°	0	R_{17}°	R_{18}°	0

 S_{ij}

$i \backslash j$	1	2	3	4	5	6	7	8	9
1	0	-1	1	1	0	1	1	1	0
2	0	1	-1	0	1	0	0	1	1
3	0	0	0	1	1	0	-1	0	0
4	1	1	1	-1	-2	0	1	-1	0

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13. ABSTRACT A simplified technique for solving "stiff" differential equations common to chemically reacting quasi-one-dimensional inviscid non-equilibrium flow analyses is presented. The method is basically that used by Degroat and Abbett with the generalization made to allow for a prescribed area distribution rather than the constant pressure (and hence constant velocity) process assumed by them. In addition, the equations are written for hydrogen/air combustion rather than methane/air. The advantage of the technique is that the chemical kinetic calculations can be solved quickly without loss of accuracy, and thus can be relegated to the status of a subroutine in complicated fluid-dynamic problems.			

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